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THE POLLUTION HAZARD ASSESSMENT SYSTEM:
DOCUMENTATION AND USERS MANUAL

MITCHELL J. SMALL

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JAN 19 1990
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PREFACE

This report documents computer software developed under Work Unit 686 (Hazard Assessment Method Computerization) in the Environmental Quality Research Branch of the Health Effects Research Division.

The author acknowledges the support of Jesse J. Barkley, Jr., Branch Chief, and the suggestions of Dr. David H. Rosenblatt, developer of the Preliminary Pollutant Limit Value approach. The author also acknowledges the technical review of Mr. Jeffry D. Leach and Dr. Winifred G. Palmer.

The Defense Technical Information Center does not supply software. The author will supply the software if you provide two unmarked two-sided double-density 5-1/4 inch floppy disks and a suitable mailer. Send disks to

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<p>The Preliminary Pollutant Limit Value approach has been used for assessments of soil and water contamination at several U.S. Army installations. This report documents the adaptation of this approach into a software computer package, the Pollution Hazard Assessment System (PHAS). PHAS has been programmed in BASIC code, which is capable of being handled on many personal computer configurations, and can be supported with a system with 640K memory, two-disk drives, a monochrome monitor, and a line printer.</p> <p>PHAS has been prepared in modular form. The user is guided through the system with menu displays in a user-friendly format. The user can prepare information for immediate analysis, or store information in off-line files for recall. Files can be recalled for analysis or</p>					
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modification. Three set of user files are employed: files which store information about scenario pathways of human exposure; files which store data about human intake, livestock characteristics (for human consumption of beef or milk), and site-specific factors; and files which store information about chemical-specific properties. The user can select up to eight exposure pathways for water-based contamination problems or fourteen exposure pathways for soil-based contamination problems. A chemical estimation module is provided to assist the user in developing data for chemicals. This module can be used in conjunction with the rest of the system or as a stand-alone routine.

The main text provides the user with system instructions. Appendix A presents the source code along with commentary. Appendix B presents the PPLV equations adapted for use in PHAS. Appendix C discusses the values assigned for human, livestock, and site-specific data elements.

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1.0 INTRODUCTION

This Pollution Hazard Assessment System (PHAS) is a suite of programs used to calculate acceptable site-specific soil or water pollutant levels from which decisions can be made about the degree of hazard at a site. PHAS performs this task by a modification of the Preliminary Pollutant Limit Value (PPLV) approach¹ as described by Small². PHAS allows users to create data files for site-specific and chemical-specific data. It includes a group of techniques to provide estimates of chemical property inputs to PPLV calculations when experimental values are not available in the literature. The present version of PHAS is designed for use on the IBM Personal Computer (PC), its family of successors, and compatibles.

This document describes PHAS and is intended to serve, in part, as a user's manual. The general assessment problem and the PPLV approach to its resolution is discussed in Section 2.0. This helps the reader to understand the system's response to the assessment problem. The system is reviewed in Section 3.0, first as a whole, and then in terms of component programs. Operations are presented at two levels. Section 4.0 presents instructions for use of PHAS. Section 5.0 presents instructions for chemical estimation subroutines that can be employed in conjunction with PHAS. These two sections comprise the "user's manual" of PHAS and cover the "how" and "when" aspects of system programs. A second level of description is provided for persons interested in system structure, thus Appendix A presents PHAS program code and commentaries on execution. Appendices B and C respectively provide the equations for PPLV evaluation and a discussion of initial input data. The present document relies on reference 2 for the bulk of the technical PPLV approach details, which contains much background and explanation not provided in the Appendices.

2.0 THE PPLV APPROACH TO HAZARD ASSESSMENT

The US Army owns property contaminated with chemical agents, munitions, explosives, smoke residues, solvents, paints, or their environmental by-products. The contamination occurs in soil, surface water, or groundwater. Decisions need to be made as to whether remedial actions are required to reduce the amount or extent of contamination, despite often insufficient information concerning the contaminants. These decisions may be internally directed by the Army or may be in response to regulations of either the Comprehensive Environmental Response, Compensation and Liability Act of 1980³, including 1986 amendments (commonly called "Superfund"), or the Resource Conservation and Recovery Act⁴.

The PPLV approach has been developed and refined at the US Army Biomedical Research and Development Laboratory. It provides answers to the "How Clean is Clean?" question, which is central to determining the need for, or the extent of, remedial actions. The approach can be used for such applications as determining sensitivity objectives in investigative survey sampling or for setting remedial action target levels.

The PPLV approach is based on linking soil or water contamination levels to an acceptable intake, which if attained, either through direct exposure to soil

or water or through consumption of foodstuffs raised or grown on a contaminated site, does not pose a hazard to the exposed population. For the present overview, sites will be discussed in terms of soil contamination. The approach consists of the following steps:

- o Determine the pollutants of concern.
- o Determine land-use scenarios and component pathways through which people are exposed to the pollutants.
- o Develop an equation for each pathway that relates the human intake of a substance to its concentration in soil.
- o Collect data needed to solve such equations.
- o For each pollutant and scenario, compute the soil limits for individual pathways, and from these, calculate a PPLV.
- o Interpret the results, and
- o Determine if other considerations (such as aquatic toxicity) might indicate that limits lower than the PPLV should be applied.

The first two steps in the PPLV approach answer the questions "What are the contaminants and how will people be exposed to them?". Often, a list of substances purchased or produced during active production is available. One should not accept such a list without question. Certain substances, such as gases or extremely volatile liquids, can easily be eliminated. Derived compounds or by-products may have to be added. The presence of naturally occurring or ubiquitous substances must be addressed. The prudent approach is to sample and analyze for all suspected soil pollutants. In "Superfund"-related actions, this is part of the Remedial Investigation. The PPLV approach can provide guidance to target analytical limits.

In the second step, land-use scenarios are defined in terms of current or projected activities at or near an installation. Each scenario will have one or more pathways associated with it. The pathways describe specific routes by which people can be exposed to a soil pollutant. For example, suppose that a contaminated site on an installation includes a pond designated for recreational purposes. If the pond is used for fishing and there is run-off to the pond from contaminated soils, a soil → water → fish → human pathway should be addressed. If there is a picnic and play area at the site, one might expect that children could inadvertently ingest soil. Then, a direct soil → human pathway would be included in the scenario.

For each proposed pathway, an equation is developed to describe the relation between human intake and the pollutant level in soil. The PPLV approach first processes each pathway as if it were the only pathway for a soil contaminant to reach man. The human intake of interest (units of mg/day) is based on a "safe" or "acceptable" contaminant dose. This dose (units of mg/kg-day) is given the symbol D_T . The computed soil concentration is called as a "Single-Pathway Limit Value" or SPLV.

SPLV relations have the general symbolic form:

$$\text{SPLV}_i = \text{BW} \times D_T / (\text{IF}_i \times f(\text{K}_i, \text{S}_i)) \quad (1)$$

where i refers to a specific pathway. IF_i is an "intake factor", that typically includes information about the ingestion rate of food, water or air. BW is a representative body weight for a hypothetical exposed individual. The functional term $f(\text{K}_i, \text{S}_i)$ is a measure of the ability of a pollutant to be transmitted from soil to the ingested item (if the item ingested is soil itself, this function is unity). K_i usually includes one or more partition coefficients, numbers that indicate the relative pollutant concentration in adjacent portions of a pathway. In the fish pathway discussed above, the fish bioconcentration factor (BCF) relates the quasi-equilibrium concentrations in water and fish. S_i involves site-specific information about soil.

The next step is to calculate the PPLV for each land-use scenario. The PPLV is usually computed from the component pathway SPLVs of a scenario:

$$\text{PPLV} = 1 / \sum_i (\text{SPLV}_i)^{-1} \quad (2)$$

The above relation is valid when all exposure to a pollutant is described by the pathway equations and the $f(\text{K}_i, \text{S}_i)$ do not vary with concentration.

While the approach described above addresses adverse effects in humans, there is no guarantee that a PPLV would be a safe limit for other species of concern. This must be considered in a complete analysis. Should the PPLV exceed a soil or water concentration that could cause unacceptable adverse effects to other biota, or lead to aesthetic problems, a "Type 1" constraint is said to occur. A second contingency to be addressed is that the physicochemical properties of a pollutant, particularly water solubility, could preclude a dose of magnitude D_T from being attained at the PPLV. If this occurs (a "Type 2" constraint), a soil level in excess of the calculated PPLV could be acceptable.

PHAS uses "unit contamination" equations to compute PPLVs. The equations assume either 1 mg pollutant/kg soil or 1 mg pollutant/L water. For each pathway, the equation determines exposure resulting from the presence of a unit concentration of pollutant in soil or water. The sum of these intakes, I_m (units mg/day per unit concentration), can be contrasted to a limiting intake $\text{BW} \times D_T$, from which the PPLV is computed:

$$\text{PPLV} = \text{BW} \times D_T / \text{I}_m \quad (3)$$

To demonstrate the agreement between equations (2) and (3), the SPLV relation of equation (1) can be recast as:

$$\text{SPLV} = \text{BW} \times D_T / R_i \quad (4)$$

If this is inserted in equation (2), the following is obtained:

$$\text{PPLV} = \text{BW} \times D_T / \sum_i R_i \quad (5)$$

From (3) and (5), $I_m = \sum_i R_i$. The R_i are seen to be pathway intakes associated with unit contamination. R_i values can be obtained from previously-developed SPLV equations; from the symbolic notation of equation 1,

$$R_i = I_{Fi} \times f(K_i, S_i)$$

3.0 DESCRIPTION OF PHAS STRUCTURE

3.1 Hardware

You will need a PC or compatible computer system with 640 K capacity, a MS-DOS operation system of level 3.1 or higher, along with either GW-BASIC* or IBM BASICA* software. PHAS will run on a system with either two floppy disk drives or a floppy disk-hard disk drive configuration. A printer with 8.5-inch wide paper is required, and, as a minimum, an 80-column wide monochrome monitor.

PHAS is supplied on two 5-1/4 inch floppy disks (see Preface). The first disk (Disk 1) contains phas programs and read-only data files. The second disk (Disk 2) contains external files for the storage of scenario definitions and the storage of variables used in assessment computations. The programs are supplied in source BASIC code; the program codes appear and are explained in Appendix A.

3.2 System Structure and External Files

PHAS is designed to store information about human weight, consumption patterns, livestock weight and consumption data, site characteristics, as well as the physical-chemical, environmental transfer, and toxicological properties of substances in external files. These files can be created at one time and recalled for use at another time. Three specific types of files are used; they are differentiated by their filename extension. You will have to know these to run your analyses. The extensions will be used in the text for reference:

- | | |
|-----------|--|
| .PTH File | This file stores two index lists. The first keeps track of pathways involved in a given scenario, and includes 30 elements. The second is a coded index describing the role of data in PPLV calculations, and includes 140 elements. It is called the Data Use Status Table (DUST). This file also stores one alphanumeric entry, which is either 'soil' or 'water'. |
| .LDS File | This file contains 90 numeric entries. The entries are the non-chemical specific information inputs in a PPLV analysis, including human and livestock consumption factors and site soil characteristics. |

* In the text, availability of GW-BASIC is assumed.

.DAT File This file contains 50 numeric entries and an alphanumeric entry. The numeric entries are the chemical-specific information, while the alphanumeric entry is the chemical name.

The various programs in PHAS allow you to access, modify, and store files. However, you can't use PHAS to delete files. For this purpose, you can use the DOS-provided ERASE or DELETE utilities*, or within the GW-BASIC compiler, the KILL command.

Figure 1 is a schematic of PHAS structure. Entry to and exit from PHAS is via OPEN11. With the exception of CHMPRP11, access to any other program in the structure is through OPEN11. These programs are briefly described in Figure 2 (This also appears as an advisory message accessed via OPEN11).

In PATWAY11, you do the scenario-definition phase of the assessment process. In doing so, you can create or use .PTH files. A .PTH file can be used in the two data-handling modules INPUTS11 and CHMFIL11 as a "filter", whereby only data required for assessments, or information from which such data can be

* The "SHELL" command can be used to perform these chores without exiting to DOS from GW-BASIC.

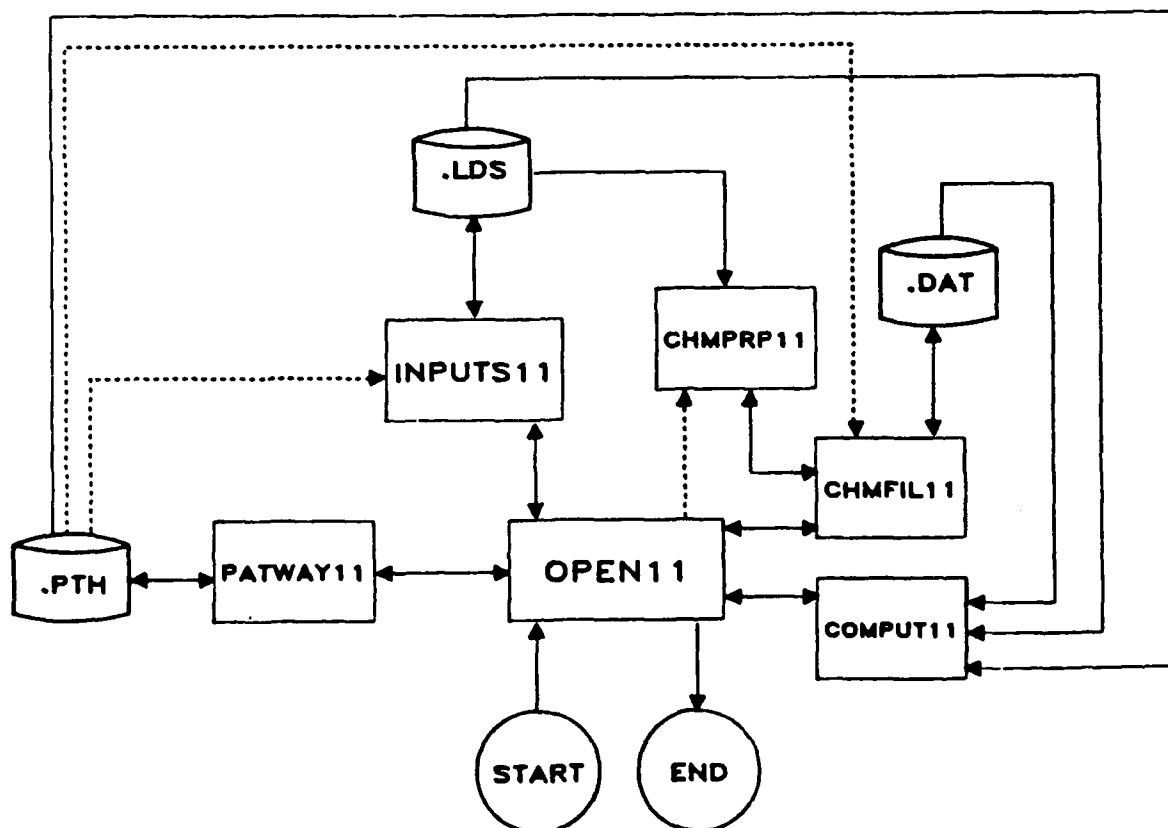


Figure 1. PHAS System Structure

***** OVERVIEW OF PHAS PROGRAM MODULES *****

PATWAY11 lets you select the exposure pathways that comprise a scenario. The module identifies non-chemical and chemical-related variables required for the analysis, and provides a planning guide to the analysis. Results can be stored in an off-line .PTH file.

INPUTS11 processes non-chemical data and creates off-line .LDS files. These files can be down-loaded and used in PPLV analyses directly or their data modified. The modified data can be stored under the name of the down-loaded file or under a new name, thereby creating a new file.

CHMFIL11 processes chemical data and creates .DAT files. These files can be down-loaded and used in PPLV analyses directly or their data modified. You can either modify down-loaded data or obtain estimates from estimation methods in CHMPRP11. Results can be stored as discussed above in the INPUTS11 paragraph.

CHMPRP11 serves two purposes. It is used by CHMFIL11 to estimate chemical properties during a chemical data processing routine. CHMPRP11 can be accessed directly from OPEN11 for 'a la carte' estimates; in this operating mode, you supply all input information.

COMPUT11 calculates PPLV results, and as an option, performs constraint analyses on the assessment to identify non-human targets that should be addressed before adopting PPLV values as criteria for clean-up guidance.

Figure 2. On-Line System Description Message

estimated, is handled. This is shown by the dashed lines directed from a .PTH file to each of these modules.

As will be noted in Sections 4.5 through 4.7, several file processing options are available, ranging from the simple down-loading of existing external files to their creation, modification, and storage on disk. These processes are indicated by the double-arrow lines connecting each file with a corresponding module. Moreover, any one of the modules can be entered from OPEN11. CHMFIL11 permits use of the module CHMPRP11 to quantitatively estimate values for data that are not available to the user from other sources.

The COMPUT11 module contains the unit concentration assessment algorithm and, as an option, performs the two constraint analyses described in Section 2.0. Data for COMPUT11 can be obtained in several different ways. At one extreme, you can simply run COMPUT11 based on data stored in .PTH, .LDS, and .DAT files; this is shown by the three lines connecting these files to the COMPUT11 module. At the other extreme, you can enter PATWAY11, INPUTS11, and CHMFIL11, develop the requisite data files in each module, and then enter COMPUT11. Once you have completed an assessment in COMPUT11, the files remain available for alteration of variables in a "what if" or sensitivity analyses.

The CHMPRP11 module includes information about and estimation methods for several chemically-related variable properties. It can be accessed through CHMFIL11, whereby the method results can be retained for system use. You can access CHMPRP11 directly from OPEN11 for operation in an "a la carte" mode, for estimating properties without storing or using results further in PHAS. When the CHMPRP11 module is accessed through CHMFIL11, data from a .DAT file is used. However, some estimation methods also require information from a .LDS file. Thus, Figure 1 shows the link from .LDS files to CHMPRP11 as a directed line.

4.0 PHAS OPERATING INSTRUCTIONS.

4.1 General System Notes

PHAS is user-friendly in several respects. It provides on-line prompts describing each subsection of a program and the inputs you need to enter. After a manual input of any kind, the return (enter) key is pressed. Your operational inputs are either integer numeric entries, alphanumeric entries, or filenames. All alphanumeric entries are in lower-case characters. Many halts are provided to permit you to print the contents of a screen display. To do this, simultaneously depress the "Shift" and the "Print-Screen" keys.

The inputs are monitored to detect common errors. When such an error occurs, you are so informed, and you can repeat the input process. Common errors include:

- * An integer input outside of the values specified.
- * A non-integer input when an integer is specified.
- * An unspecified alphanumeric input (typographical error).
- * A filename input that violates DOS specifications.
- * A filename input with a missing or incorrect extension.
- * A filename input for a non-existing file.

If you enter an alphanumeric input when a numeric input is expected, or vice versa, the compiler issues the message "?Redo from start". If this happens, check your input and enter the corrected information (followed by a return).

Specific conventions are followed in the instructions. Modules, file extensions, and specific file names are shown in capital letters. Direct passages from the system are in compressed pitch font (compressed pitch font) and either in full quotes within the text or set apart from the text. Inputs to the system are shown in single quotes; in practice, they are entered without quotation marks, and are concluded by pressing the return (enter) key. The term "current session" refers to all transactions from start of execution of OPEN11 to the present instant. The term "on-line storage" refers to information currently stored in computer memory; the information may also be stored on a floppy or hard disk. The term "down-load" means to transfer information from a file on an external storage device for use in one or more PHAS modules. Several paragraphs and sections discuss PHAS arrangement of data elements. These passages can be omitted in initial readings and then read after you gain some confidence with PHAS operation. They are preceded by a double asterisk (**).

4.2 Installing PHAS

You should copy issued PHAS disks (see Preface) for day-to-day operations or for installation purposes. The issued disks can then be stored. Figure 3 shows PHAS files supplied on Disk 1. As a minimum, the files PROMPT.CMP, DEFALVA.LDS, DEFALVC.LDS, DEFALC.DAT, S036AC.PTH and DEFAULT.PTH are provided on Disk 2. Other .DAT files (information on specific compounds prepared by the author) and .DOC files (documentation for these files) are also on Disk 2.

Volume in drive A has no label
Directory of A:\

INSTALL	BAS	COMPUT11	BAS	CHMPRP11	BAS	OPEN11	BAS	PATHWAY	CMP
CHMFIL11	BAS	PATWAY11	BAS	INPUTS11	BAS	PATPMP	CMP	VFFACTOR	CMP
WILTBOIL	CMP	STOREIT	CMP	VAPMENU	CMP	KPATINFO	CMP	MILLERM	CMP
KOCINFO	CMP	DTINFO1	CMP	KPMINFO	CMP	TMELT	CMP	LEBAS	CMP
KSPKSV	CMP	OVERVIEW	CMP	ASSIGN	CMP	VAPRESS	CMP	COMPUTE	CMP
AQUATOX	CMP	KPDINFO	CMP	CATTOX	CMP	CATLIST	CMP	BCFINFO	CMP
CHEMFILE	CMP	CHEMPROP	CMP	CONTALK	CMP	DAINFO	CMP	DIAGNOST	CMP
DTINFO2	CMP	INPUTS	CMP	KDINFO	CMP	KWPVINFO	CMP	LOGKOW	CMP
WOLWT	CMP	ORGLEP	CMP	PERMINFO	CMP	PHYTOTOX	CMP	STATDEX	CMP
HENRY	CMP	TBOIL	CMP	VPTABLE	CMP	WATERSOL	CMP	PARAM	CMP

50 File(s) 190484 bytes free

A>

Figure 3. Listing of PHAS Files on Disk 1

The specific installation procedure depends upon your computer disk drive configuration. Here, installation is discussed for configurations the author has encountered.

4.2.1 Dual Floppy Disk Drive Operation

The files of Disk 1 (see Section 3.1) should be copied to a floppy disk containing both MS-DOS and GW-BASIC. This disk is herein called the "Execution Disk". Next, the drive in which the Disk 2 files will reside is declared. Insert the Execution Disk in disk drive "A". At the DOS prompt, type 'gwbasic install' if you have GW-BASIC; if you have BASICA, type 'basica install'.

The file INSTALL.BAS is executed (see Appendix A for details). A menu with four numeric options is displayed. For dual floppy disk operations, select option '2'. For PHAS operations, the Execution Disk is placed in the "A" drive; Disk 2 is placed in the "B" drive.

4.2.2 Virtual Disk and One Floppy Disk

You can reserve a portion of computer memory to store Disk 1 PHAS programs. This portion is called a virtual disk, and is here called the "C" drive. Prepare an Execution Disk as described above; the file VDISK.SYS (provided with IBM MS-DOS) or RAMDRIVE.SYS (provided with Microsoft MS-DOS) must be copied to this disk. The DEVICE statement in CONFIG.SYS should allocate at least 300K memory to the virtual disk. Place the Execution Disk in "A" drive, and do the INSTALL procedure discussed above, but select option "1" (this indicates that Disk 2 is to be located in the "A" drive). ISSUED PHAS DISKS ARE PRE-INSTALLED FOR THIS CONFIGURATION. Files can be copied from the Execution Disk to the "C" drive by the global COPY command ('copy a:*. * c:'). For convenience, you can prepare an AUTOEXEC.BAT file with this command.

4.2.3 Hard Disk and a Floppy Disk

This section applies if you want to put your executable programs on a hard disk. First, you create a subdirectory on the hard disk, and then you copy

the contents of Disk 1 to that subdirectory. Depending upon how your system is configured, you may have to copy a version of BASIC to that same subdirectory. In the INSTALL procedure, select option '1'. During PHAS operations, Disk 2 is placed in the "A" drive. ISSUED PHAS DISKS ARE PRE-INSTALLED FOR THIS CONFIGURATION.

4.2.4 Hard Disk

All files can be stored on a hard disk. Copy the contents of Disk 1 to a hard disk subdirectory as discussed in Section 4.2.3. You can either place PHAS in one subdirectory, or have the execution programs in one subdirectory and the external files in another. If you wish to place PHAS in one subdirectory, you select option '3' in the INSTALL procedure. After the INSTALL procedure, copy the contents of Disk 2 to that subdirectory. If you want the external files on another subdirectory of the hard disk, in the INSTALL procedure, select option '4'. You are then prompted to enter the full subdirectory name in which the contents of Disk 2 will reside*. Then copy the contents of Disk 2 to that subdirectory.

4.3 OPEN11

4.3.1. Operating Procedures

At the DOS drive prompt, enter 'gwbasic open11' if you are using GW-BASIC; if you're using BASICA, enter 'basica open11'. The module displays the main menu (Figure 4). Otherwise, an error message is displayed, indicating an error condition and the probable remedial action; see Section 4.3.2.

The main menu accepts a prompt value between 1 and 10 (except 8) to start a specific function. Entries 1 and 2 route you to monitor-displayed system and program explanations of PHAS (i.e., Figure 2 is the system explanation). If you enter '2', you encounter the display line: "SELECT FUNCTION NUMBER FOR DESIRED MODULE". Supply the option number for the desired explanation. At the conclusion of a module display, the main OPEN11 menu reappears. The input '6' is used for viewing specific on-line stored data units. Instructions for use of this option are included in Sections 4.4, 4.5, and 4.6.

Type '10' to exit PHAS. OPEN11 prevents termination due to a typing error, so you must confirm your request. A 'yes' entry is required to leave the system; a 'no' entry routes you to the selection menu.

4.3.2 Error Messages and Resolution

If INSTALL.BAS has not been executed, OPEN11 is terminated. You are advised of this condition. When applicable, another condition checked is that the Disk 2 files are in the floppy disk drive selected in the INSTALL procedure. If the drive is empty, you are advised of this, and you should proceed to

* For example, the hard drive might be the "D" drive. The files from Disk 1 have been copied to the subdirectory d:\themod11\diska\. The files from Disk 2 are to be copied to a subdirectory of "themod11" called "diskb." The entry in INSTALL.BAS is d:\themod11\diskb\.

***** POLLUTANT HAZARD ASSESSMENT SYSTEM (PHAS)*****

Version 1.1, March 1989

***** MAIN FUNCTION SELECTION MENU *****

ENTER	FUNCTION PERFORMED BY ENTRY
1	To get a brief description of the system.
2	To get a more in-depth description of specific modules.
3	To do your scenario definition and pathway selections.
4	To do your non-chemical data selection and editing.
5	To do your chemical data selection and editing.
6	To review on-line data and pathway information.
7	To do PPLV Calculation and constraint analysis.
9	To do selected Chemical Estimation Methods 'off-line'.
10	To exit the system.

ENTER YOUR FUNCTION NUMBER:

Figure 4. Main Menu of the OPEN11 Module

insert the correct disk. If a non-PHAS disk is in a floppy disk drive, replace it with the correct disk. In either case, after placing the correct disk in the drive, simply press the "enter" key in response to the "?" prompt. However, if Disk 2 files were expected in a hard disk subdirectory, this error would occur only if Disk 2 files had not been copied to that subdirectory. In this case, simultaneously depress the "Control" and "Break" keys to enter "direct mode" BASIC operations, and then type 'system' to exit to DOS. Then copy Disk 2 to the applicable subdirectory before re-starting PHAS. If you are versed in BASIC, you can use the "SHELL" command in the direct mode to invoke the DOS copy utility directly and then continue with the direct mode command 'load "open11",r '.

4.4 A Sample Problem

To illustrate PHAS operations, a sample problem is processed in subsequent sections. The scenario is as follows: There is an area of a former ammunition plant where soil is contaminated with "trinitroanything", a persistent organic compound, at levels up to 2 mg/kg. A decision is needed as to whether a 2 mg/kg level is acceptable for current land use; if not, remedial efforts may be necessary. The area is rural, consisting of small farms. The inhabitants grow most of their own vegetables, and raise cattle, primarily for their own consumption. The analyst has decided to also include "trinitroanything" intake via inhaled vapors diffusing from residential basements and the incidental intake of ingested or inhaled particles of contaminated soil.

4.5 PATWAY11

4.5.1 Running PATWAY11

You access this module by responding '3' to the Selection Menu (Figure 4) in OPEN11. The "MODE OF OPERATION SELECTION MENU" is displayed, and you are queried:

Input '1' if you are using a stored file in a 'load and go' mode ONLY.
Otherwise input '2'.

Enter '1' or '2' in response. PATWAY11, INPUTS11, and CHMFIL11 have two major modes of operation, "load and go" and file processing/storage. In the "load and go" mode, PATWAY11 down-loads a specified .PTH file and transfers control back to OPEN11. In terms of Figure 1, this process is indicated by arrows leading from a stored .PTH file through PATWAY11 to OPEN11. This mode is useful when you want to use a previously-created .PTH file to index several .LDS or .DAT files for modification purposes. This mode is also useful if you wish to review the contents of a .PTH file in storage (see Section 4.5.2).

In either operation mode, you then have the option to view the directory of .PTH files. If you respond 'yes', these files are listed.* In the "load and go" mode, this listing helps prevent you from down-loading an unwanted file or attempting to down-load a nonexistent file. If you are in the file processing/storage mode and plan to create a .PTH file for storage, you should know the current filenames to avoid an unintentional overwrite of a stored file. An overwrite will occur if you designate an existing filename for storage. On the other hand, you may want to intentionally overwrite a stored file; this is how you "modify" a .PTH file (see below). Filenames remain displayed until you select a filename for storage.

In the "load and go" mode, the module requests the name of the file to be down-loaded. If no errors occur in the filename response, the pathways included in the file are displayed. Execution pauses so you can review the display, and after the requisite 'return', program execution is transferred to OPEN11.

PATWAY11 does not modify stored .PTH files. Thus, the file processing/storage mode, which is indicated by the display "SCENARIO CONSTRUCTION ROUTINE", always starts from "scratch". First, you designate the medium of interest, either 'soil' or 'water' (in the sample problem, you would enter 'soil'). Based on this designation, the module presents the pathway repertoire one path at a time. Each pathway includes a description of what process it portrays. The description is somewhat cryptic due to space restrictions. The following rules are used; the pathway 6 and pathway 12 descriptions in Figure 5 show examples of these rules.

- * The description proceeds from left (the medium) to right (man).
- * Transfers with partition coefficients are indicated by '-->'.
- * Unless specified, oral human uptake is assumed. If another route is involved, the organ is shown in braces, such as [skin] for dermal absorption.
- * Transfers to man are indicated by '->>'.

* Users are cautioned of a system "glitch" at this step. The output is a header subdirectory (or disk) and a list of files. The header subdirectory is the one containing PATWAY11, and may NOT be the subdirectory containing the .PTH files.

* In case the pathway involves several routes to an intermediate species (particularly livestock or dairy cows), each route is indicated by a '&&&' and the intermediate species identification is bracketed.

After each pathway description, answer 'yes' or 'no' when prompted. At the conclusion of this input routine, the module checks if no pathways were selected. You may view the pathway repertoire to see its contents; in that case, all 'no' responses are logical. The module displays this message:

NO PATHWAYS WERE SELECTED IN THIS RUN. IS THIS WHAT YOU WANT?
Please enter yes or no.

If you respond 'yes', control is transferred directly to OPEN11. If you respond 'no', it repeats the entire repertoire query routine. In the sample problem, a 'yes' response would be entered for pathways 3, 6, 10, and 12 (these pathway descriptions are shown in Figure 5).

If one or more pathways have been selected, the module produces a line printer output such as shown in Figure 5. As this is prepared, the message "NOW PRINTING OUT DATA REQUIREMENTS SUMMARY" is displayed. The printed output identifies the variables which are or which may be needed to compute the PPLV for the selected pathways. With this output, you can plan a strategy for providing data inputs.

The output is divided into several sections. The first lists "global" variables, which are used in every relation. The second section describes each selected pathway, and the variables used in SPLV equations (see Appendix B). The section "COMPUTATION OPTIONS FOR CHEMICAL MAIN PATH VARIABLES" addresses chemical-specific variables that can be estimated, and goes through a summary listing of estimation routines. The routines reside in CHMPRP11. The final section, "CONSTRAINT ANALYSIS ADVISORY" indicates possible "type 1" and "type 2" constraints that may affect the usefulness of the PPLV as an assessment criterion.

At the conclusion of this printout, you enter the "STORAGE DISPOSITION MENU" where you are given the option to retain the scenario developed in external storage. If you respond '1', this option is declined. If you respond '2', you are prompted for a filename of up to 8 alphanumeric characters. The filename must meet DOS specifications, and this prompt will be repeated if there are errors (period alphanumeric or too many characters). Remember that files are not write-protected; you will have to exercise care to prevent unwanted replacement of a stored file.

The output from PATWAY11 (either the contents of a down-loaded file or a created scenario) resides in on-line storage and remains there until you either (1) down-load another .PTH file in PATWAY11 or in COMPUT11, or (2) create another scenario in PATWAY11.

4.5.2 .PTH Files

Two .PTH files are on Disk 2, DEFAULT.PTH and S036AC.PTH. One .PTH file must be stored on disk at all times. S036AC.PTH is the file for the sample problem.

***** PATHWAY SELECTIONS AND DATA NEEDS SUMMARY *****

FOR ALL PATHWAYS. YOU WILL NEED

Adult body weight, kg [BW] or Child body weight, kg [BWc]
and either
Long term no-effect human dose, mg/kg-day [DT]
or Shorter term no-effect human dose, mg/kg-day [DTc]

***** SPECIAL ABBREVIATIONS *****

dwb = dry weight basis
nodim = dimensionless
p.c. = partition coefficient

PATHWAY 3 eat contaminated vegetables grown in soil.
SOIL-->SOIL PORE WATER-->VEGS-->MAN.

PRIME VARIABLES INVOLVED IN CALCULATION ARE
Representative vegetable intake, kg dwb/day [Wv]
Adjustment for less than representative vegetable intake [SWv]
Surface soil nominal density, kg/L [rh1]
Surface soil moisture content, fraction [th1]
Water to vegetable partition coefficient, L/kg dwb [Kwv]
Soil to water partition coefficient, surface soil, L/kg [Kd1]

PATHWAY 6 eat beef; cattle graze on plants in contaminated soil, ingest soil
and drink contaminated water. SOIL-->SOIL PORE WATER-->PLANT-->\$\$\$
SOIL-->\$\$\$ SOIL-->WATER-->[COW(beef)]-->MAN.

PRIME VARIABLES INVOLVED IN CALCULATION ARE
Representative beef intake, kg/day [Wb]
Adjustment for less than representative beef intake [SWb]
Steer uptake of water, L/day [Uwm]
Steer uptake of forage, kg dwb/day [Uom]
Steer incidental uptake of soil in forage, kg/day [Usm]
Surface soil nominal density, kg/L [rh1]
Surface soil moisture content, fraction [th1]
Drinking water body sediment nominal density, kg/L [rh2]
Drinking water body sediment moisture content [th2]
Water to forage partition coefficient, L/kg dwb forage [Kwo]
Plant to beef partition coefficient, kg dwb forage/kg meat [Kpm]
Soil to water partition coefficient, surface soil, L/kg [Kd1]
Soil to water partition coefficient, pathway 12, L/kg [Kd2]

PATHWAY 10 intake of contaminated soil by combined ingestion, inhalation or
skin absorption under 'normal' lifestyle conditions. SOIL-->MAN.

PRIME VARIABLES INVOLVED IN CALCULATION ARE
Incidental soil ingestion rate, normal conditions, kg/day [Wsn]
Adjustment for non-model exposure to soil/dust [SWsn]

PATHWAY 12 inhalation of vapors from soil surrounding enclosed space,
such as a basement. SOIL-->SOIL PORE AIR-->[lungs]MAN.

PRIME VARIABLES INVOLVED IN CALCULATION ARE
Inhalation rate, enclosed area vapor model, m³/day [Rb]
Adjustment for tenure in enclosed area vapor model [SRb]
Vapor-laden soil representative bulk density, kg/L [rh3]
Vapor-laden soil representative moisture content [th3]
Vapor-laden soil representative void fraction [ep3]
Volume-area ratio of basement (or other enclosure), m [VAR]
Time per air change factor for enclosure vapor path, days [TAC]
Initial time of analysis (entry), basement diffusion case, day [TDb]
End time of analysis, basement diffusion case, day [TLb]
Henry Law constant, dimensionless [Kh]
Molecular diffusivity in air, m²/day [Da]
Soil to water partition coefficient, surface/subsurface soil, L/kg [Kd3]

Figure 5. Scenario Description and Input Options, Sample Problem
(page 1 of 3 pages).

*****COMPUTATION OPTIONS FOR CHEMICAL MAIN PATH VARIABLES*****

Water to vegetable partition coefficient, L/kg dwb [Kwv]
 can be estimated by three methods in PHAS. First,
 $Kwv = \text{Water to forage partition coefficient, L/kg dwb forage [Kwo]}$
 Second, Kwv is function of
 Log octanol-water partition coefficient [LogKow]
 Third, Kwv can be estimated from
 Soil to forage partition coefficient, kg soil/kg dwb forage [Kso]
 or Soil to vegetable partition coefficient, kg soil/kg dwb [Ksv]
 If soil-water partition coefficient info is available about soil
 used to characterize Ksv or Ksp [Kd(soil)],
 $Kwv = Ksv \times Kd(\text{soil})$ or $Ksp \times Kd(\text{soil})$
 See Kd2 message for estimation methods of Kd(soil)

NOTE: Kwp can be estimated by analog, replacing Kwv for Kwo
 above and vice versa.
 Kd2 message for estimation methods applicable to all Kd.

Soil to water partition coefficient, pathway 12, L/kg [Kd2]
 $= Koc \times foc + (th2/rh2)$

Soil organic carbon from water partition coefficient, L water/kg OC [Koc]
 can be estimated as a function of
 Water solubility, mg/L [SW]
 or Log octanol-water partition coefficient [LogKow]

Plant to beef partition coefficient, kg dwb forage/kg meat [Kpm]
 can be estimated by two methods. First, $Kpm = Kpat \times fm$
 where
 Forage to meat fat part. coefficient, kg dwb forage/kg adipose tissue [Kpat]
 Fat content of beef, fraction [fm]

Next, $Kpm = Kpd \times (fm/fd)$, where
 Plant to dairy partition coefficient, kg dwb forage/L milk [Kod]
 Fat content of milk, fraction [fd]

Kpat can be estimated as a function of
 Water solubility, mg/L [SW]
 or Log octanol-water partition coefficient [LogKow]

Henry Law constant, dimensionless [Kh]
 may be estimated by the quotient of
 Saturated vapor pressure, mm Hg [VP] divided by
 Water solubility, mg/L [SW]

Several estimation methods are available for each of these.
 Water solubility can be estimated from
 Log octanol-water partition coefficient [LogKow]
 Vapor pressure can be estimated from
 Normal or extrapolated boiling point, deg C [Tboil]
 For liquids. Generally for solids.
 Normal or extrapolated melting point, deg C [Tmelt]
 will be needed. Check CHMPRP11 for more details.

Molecular diffusivity in air, m^2/day [Da]
 can be estimated from molecular components and
 Molecular weight, g/gmol [MW]

Kd2 message for estimation methods applicable to all Kd.

See Kd2 for estimation approaches to
 Soil to water partition coefficient, surface/subsurface soil, L/kg [Kd3]
 Substitute subscript '3' for '2'.

Figure 5. Scenario Description and Input Options, Sample Problem
 (page 2 of 3 pages).

***** CONSTRAINT ANALYSIS ADVISORY *****
 Type 1: PPLV may adversely effect non-human species or overlook
 non-toxic adverse human responses

PPLV may have adverse livestock effect constraint if
 Acceptable limit dose to cattle, mg/kg-day is in .dat file

PPLV may have phytotoxic effect constraint if
 Phytotoxic limit in hydroponic solution, mg/L or
 Phytotoxic limit in soil, mg/kg is in .dat file

Type 2 constraint occurs if conc. in water phase when soil conc.=PPLV
 Exceeds Water solubility, mg/L [SW]

Figure 5. Scenario Description and Input Options, Sample Problem
 (page 3 of 3 pages).

4.5.3 (**) VIEWING .PTH FILES

After you have returned to OPEN11, the .PTH file contents may be viewed. At the main menu (Figure 4), select option 6. You will be transferred to the "DISPLAY-PRINT UTILITY MENU". If you select option 1, you can view the pathway selected; Figure 6a shows selections (from S036AC.PTH) for the sample problem. The water-specific paths appear in the first column. The other two columns are reserved for soil pathways. Paths in a scenario are indicated by the "1" entry in Figure 6a; otherwise, "0" appears. As examples, pathway 3 is indicated by the "1" entry in the "Soil #1" column, third row; pathway 12 is indicated by the "1" entry in the "Soil #2" column, second row.

If you select option 2 at the "DISPLAY-PRINT UTILITY MENU", you can view the data use status table (DUST) for variables; Figure 6b shows the DUST for the sample problem. Each variable that can be used in any manner in PHAS is indexed from 1 to 140. The current index assignments for these variable are shown in Table 1. In the example shown in Figure 6b, the 44th item is Upm, which represents daily plant uptake by a steer. Each variable is assigned a use status code in the DUST of either '0', '1', '2', '3', or '4'. The codes translate as follows:

Code	Meaning
0	Variable is not needed for scenario processing.
1	Variable is in an equation used in scenario processing.
2	Variable is not in an equation used in scenario processing, but may be used to estimate data which is.
3	Variable has dual uses; see code 1 and 2.
4	Variable is used only in Type 1 constraint analysis.

```

***** DISPLAY-PRINT UTILITY MENU *****
Input number for desired printout
Select '1' for pathway status
Select '2' for data use status table (DUST)
Select '3' for values of non-chemical data from .LDS file
Select '4' for values of chemical data from .DAT file
Select '5' for printout of variables from .LDS and .DAT files
with narrative identities supplied.
Select '6' to quit this utility and return to main menu.

```

```

? 1
      Water      Soil #1  Soil #2
      Paths      Paths    Paths
1      0          0        0
2      0          0        1
3      0          1        0
4      0          0        0
5      0          0        0
6      0          1        0
7      0          0        0
8      0          0        0
9      0          0        0
10     0          1        0

```

1st column corresponds to water pathways 1 thru 10.
 2d column corresponds to soils pathways 1 thru 10.
 3d column corresponds to soils pathways 11 thru 20.
 Current info is from loaded or stored file ...so36ac.pth
 If no file, your on-line data is not stored off-line.
 Hit enter (return) to continue....

a. Pathways Involved

```

***** DISPLAY-PRINT UTILITY MENU *****
Input number for desired printout
Select '1' for pathway status
Select '2' for data use status table (DUST)
Select '3' for values of non-chemical data from .LDS file
Select '4' for values of chemical data from .DAT file
Select '5' for printout of variables from .LDS and .DAT files
with narrative identities supplied.
Select '6' to quit this utility and return to main menu.

```

```

? 2
eten eten+1 eten+2 eten+3 eten+4 eten+5 eten+6 eten+7 eten+8 eten+9 eten+10
(row)
0      1      1      0      0      1      1      0      1      0      1
1      0      0      0      0      0      0      0      0      0      0
2      0      0      0      0      1      1      0      1      0      1
3      0      0      0      0      0      0      0      0      0      0
4      2      2      1      1      1      0      0      0      4      0
5      0      0      0      0      0      2      1      1      0      0
6      2      1      1      0      2      1      1      1      0      0
7      0      0      0      0      0      1      1      1      0      1
8      1      0      0      0      0      0      0      0      0      0
9      2      2      2      2      2      2      0      0      0      0
10     2      2      2      2      2      2      0      0      0      0
11     0      3      3      1      2      1      1      1      1      1
12     0      0      0      0      0      1      1      0      0      0
13     0      0      4      4      4      4      0      0      0      0

```

For data index, read down for tens, add across for units.
 Thus, item at row 4, eten+4 (44) is index for Upm (see manual Table 1)
 Hit enter (return) to continue....

b. DUST for Variables

Figure 6. Stored PATWAY11-Created Indices in PHAS - Sample Problem Scenario

4.5.4 Sources of Pathways Used in PHAS

The current version of PHAS has 8 water pathways and 14 soil pathway options. The first 7 water pathways and 13 soil pathway equations were presented recently by Small². Table 2 presents a cross-reference between the pathways here and their location in the cited document². That document should be consulted for particulars of pathway assumptions involved. The last water and soil pathways deal with dermal exposure to a pollutant in water, as a result of showering, bathing, or swimming in contaminated water. They were based upon a pathway discussed in the current "Superfund Exposure Assessment Manual"⁵. The Manual's presentation⁵ is directly used for the water pathway. The soil pathway provides for the transfer of contaminant from soil to water.

(**) The equations in terms of variable names cited in Table 1 appear in Appendix B. Appendix B also lists these variables with more detailed descriptions than is provided in Table 1, along with the dimensional units used in PHAS.

4.6 INPUTS11

4.6.1 Running INPUTS11

INPUTS11 is accessed from OPEN11 by responding '4' to the Selection Menu (see Figure 4). This module and CHMFIL11 are quite similar in construction. Unlike PATWAY11, both modules require either an on-line or stored file to be available at the start of processing. This is noted in the initial message of the "MAJOR MODE OF OPERATION MENU":

Select '1' to process on-line information (in program memory)
Select '2' to use a stored .LDS file in a 'load and go' mode.
Select '3' to modify a stored .LDS file.

Selection '1' is most useful when you are making "what-if" changes to the data in a non-chemical data base for multiple analyses. On-line information is available if a .LDS file has been previously down-loaded, either in INPUTS11, COMPUT11 (See Section 4.8), or in CHMPRP11 (See Section 5.2.9).

Use selection '2' if you wish to down-load an existing database without change. This selection can also be used to select a file for review in the diagnostic selection option of OPEN11 (see Section 4.6.3). Use selection '3' to create a new .LDS file, which involves down-loading an existing stored file, possibly changing data values, and storing the values under a different filename. You can also use selection '3' to modify a stored .LDS file, which involves down-loading that file, changing data values, and storing the values under the same filename.

If you make selection '1' and there is no on-line information, you are routed back to the selection menu. Otherwise, you are advised of the last down-loaded file and given the option to continue. If you choose not to continue, you are routed back to the selection menu.

VARIABLE	VAR. INDEX	VARIABLE	VAR. INDEX
****Human Factors		****Diffusion paths parameters	
BW (Adult Body Weight)	1	VAR(volume-area ratio)	76
BWc(Child Body Weight)	2	TAC(time per air change)	77
Ww(Water Intake)	3	VW(wind velocity)	78
Wf(Fish Intake)	4	MH(Site mixing height)	79
Wv(Vegetable Intake)	5	TOb(Init anal. time[basem't])	80
Wm(Meat Intake)	6	TLb(end anal. time[basem't])	81
Wd(Milk Intake)	7	LS(Length of site)	82
Wsn(Normal Soil Intake)	8	TDo(Init anal. time[outside])	83
Wscw(Dusty-area soil Intake)	9	TLo(end anal. time [outside])	84
Rb(Enclosed area breath rate)	10	****Chem-specific estimators	
Rw(Worker breath rate)	11	MW(Molecular Weight)	91
AV(Body surface area)	12	Tmelt(Melting Point degC)	92
Teff(dermal exposure time)	13	Tboil(Boilng point degC)	93
SWw(Water Intake adjustment)	23	Log Kow	94
SWf(Fish Intake adjustment)	24	WS(Water solubility limit)	95
SWv(Veg Intake adjustment)	25	VP(Vapor pressure)	96
SWm(Meat Intake adjustment)	26	Koc(SOC-water p.c.)	101
SWd(Dairy Intake adjustment)	27	Ksp(Soil-plant p.c.)	102
SWsn(Soil exposure adjustment)	28	Ksv(Soil-veg p.c.)	103
SWscw(Dusty-area adjustment)	29	foc(ref for Ksp)	104
SRb(Basement model adjustment)	30	foc(ref for Ksv)	105
SRw(Open area model adjustment)	31	Kpat(Plant-fatty tissue p.c.)	106
SAV(Dermal exposure adjust.)	33	****Chem-specific equation variables	
****Cattle Factors		BCF(Bioconcentration factor)	111
fm(fat content of beef)	41	Kwv(Water-veg p.c.)	112
fd(fat content of milk)	42	Kwp(Water-plant p.c.)	113
Uwm(water Intake by steer)	43	Kpm(Plant-meat p.c.)	114
Upm(plant Intake by steer)	44	Kpd(Plant-milk p.c.)	115
Usm(soil Intake by steer)	45	Kh(Henry Law constant)	116
Uwd(water Intake by dairycow)	46	Da(Air diffusivity coeff.)	117
Upd(plant Intake by dairycow)	47	Kd1(Surface soil-water p.c.)	118
Ud(soil Intake by dairycow)	48	Kd2(Sediment soil-water p.c.)	119
Body weight of steer	49	Kd3(Sur/subsur soil-water p.c.)	120
Body weight of dairycow	50	PC(Dermal perm. constant)	121
****Site Factors		DT(Chronic limit dose)	126
foc1(foc surface soil)	56	DTc(Short term limit dose)	127
rh1(bulk density surf. soil)	57	****Constraint Data	
th1(moisture surface soil)	58	Organoleptic constraint	131
f(S1)(dilution factor path 1)	59	Aquatic tox constraint	132
f(S2)(dilution factor path 2)	60	Cattle tox constraint	133
foc2(foc sediment soil)	61	Phytotox constraint (water)	134
rh2(bulk density sed. soil)	62	Phytotox constraint (soil)	135
th2(moisture sed. soil)	63	foc (ref for phytotox soil)	136
ep1(air porosity surf. soil)	64		
foc3(foc sur/subsur soil)	65	NOTE: See Table B-2 for a	
rh3(bulk density " ")	66	more detailed explanation of	
th3(moisture " ")	67	symbols.	
ep3(air porosity " ")	68		

Table 1. Variable Symbols and Index Assignments in the Data Use Status Table

Table 2. Sources of Pathways in PHAS

Description	Medium and Identification	Location in Reference
Domestic water consumption	Water #1 Soil #1	2, equation 7 2, equation 15
Fish consumption	Water #2 Soil #2	2, equation 8 2, equation 16
Vegetable consumption	Water #3 Soil #3*	2, equation 9 2, equation 17
Beef consumption, pollutant in:		
drinking water only	Water #4	2, equation 10
pasture only	Soil #4	2, equation 18
pasture and water	Water #5	2, equation 11
pasture and soil	Soil #5	2, equation 19
pasture, soil, and water	Soil #6*	2, equation 20
Milk consumption, pollutant in:		
drinking water only	Water #6	2, equation 12
pasture only	Soil #7	2, equation 21
pasture and water	Water #7	2, equation 13
pasture and soil	Soil #8	2, equation 22
pasture, soil, and water	Soil #9	2, equation 23
Exposure to normal dust levels (combined ingestion, inhalation and skin absorption)	Soil #10*	2, equation 24
Exposure to construction-site levels of dust (combined as above)	Soil #11	2, equation 25
Exposure to vapors diffusing from soil:		
in confined area	Soil #12*	2, eqtns. 26, 28-30
in open area	Soil #13	2, eqtns. 27-30
Dermal absorption to skin from water	Water #8 Soil #14	5, Appendix A, Section 2.2

* These pathways are used in sample printout shown in Figure 5

With the other two selection options, you can choose to view .LDS files in storage and the comments in the PATWAY11 description are applicable here. Then you are given the option to down-load the default file. This option is useful when you want to develop a new .LDS file; the default file is a starting point. If this option is chosen (by a 'yes' response), the file DEFALVA.LDS is down-loaded without further prompting. Otherwise (after a 'no' response), you enter the name of a file to be down-loaded.

If you select the 'load and go' mode, the designated file is down-loaded and control returned to OPEN11. Otherwise, the "DATA USE STATUS TABLE (DUST) LOADING PROCESS MENU" is presented with three selection options:

- Select '1' to use the on-line scenario DUST.
- Select '2' to use the DUST from a stored '.PTH' file.
The program will prompt you for a file name.
- Select '3' to create a new file for storage or peruse all data in a .LDS file. Enter selection:

Each variable listed in Table 1 must be assigned a numerical value. However, for a given scenario, not every variable is required. The DUST limits the modification process to only those variables potentially relevant to a given scenario. If you select option '1', the on-line stored DUST is accessed. If you select option '2', the DUST from a .PTH file to be specified will be used. Option '3' allows you to access all data in the down-loaded .LDS file.

If you select option '1' but there is no valid on-line scenario information, you will be sent back for another option. If you choose option '2', you get the opportunity to see a list of .PTH files, after which you enter the desired filename. Note that if you select this option, the down-loaded information from the selected .PTH file will NOT be in on-line storage after you exit INPUTS11 (see Appendix A.5 for more details).

After the DUST is selected, the data handling section is announced by the message "DATA REVIEW AND MODIFICATION ROUTINE". From this point, the module proceeds in a similar manner with all index options. Each data item title is displayed with the current numerical value and the role of the data in the scenario analysis. You are queried:

- " Enter '1' to accept current value and move on to next variable"
- " Enter '2' to change value. Enter choice..."

If you respond with '1', the next data entry indicated by the DUST is accessed. If you respond '2,' you are prompted to enter a revised value. After this, the current information is re-displayed for your confirmation.

At the conclusion of this routine, you reach the "STORAGE DISPOSITION MENU". Three options are presented to you. If you choose option '0,' data are stored only on-line. If you choose option '1,' the on-line stored data are written to the file down-loaded at the start of the current INPUTS11 module process (an existing .LDS file is modified). If you choose option '2,' you are prompted to provide a filename for storage. If option '1' or option '2' is selected, storage occurs, and the filename is echoed back to you. With any of

these options, the data base at the end of the INPUTS11 session is in on-line storage (see above). The data base remains in on-line storage unless one of the following occurs:

- o You exit PHAS.
- o You subsequently down-load another .LDS file in the INPUTS11, COMPUT11 or CHMPRP11 module.

4.6.2 .LDS Files

Two default .LDS files are provided on Disk 2, DEFALVA.LDS and DEFALVC.LDS. These files should not be changed; PHAS will prevent you from storing a modified data base with these filenames. When you set up a .LDS file, don't replace non-zero values supplied in DEFALVA.LDS or DEFALVC.LDS with zeros for "don't know" or "don't care" variables.

(**) Table 1 identifies all variables involved in PHAS calculations. The items indexed from 1 to 90 are processed in INPUTS11. Items 1-13 deal with human factors such as body weight and consumption rates. The values presented in DEFALVC.LDS are for children while those in DEFALVA.LDS are for adults. The values in these files were developed by Small², and are representative values for adults (or children). In particular, the values chosen for the consumption variables (Ww, Wf etc.) are based on a substantial degree of intake supplied via the chosen pathways. However, the intakes are usually on a per-capita basis (for example, the vegetable intake [0.034 kg/day, dry weight] assumes that a majority of the vegetables would come from gardens, and that the target person does not eat more vegetables than would a per-capita person.) If you prepare .LDS files, corresponding sets of .LDS files should be prepared for both adults and children; the intake-to-body-weight ratio for children can be much higher than for adults.

(**) Variable items indexed from 23-31 and 33 can be used to "adjust" variables indexed from 3-11, and 13 for conditions different for those from which they were derived. These factors are set to unity in DEFALVC.LDS and DEFALVA.LDS. The first five involve consumption of water and food, and their determination is straightforward (based on the consumption for the pathway you select as contrasted to the values provided). The others are more complex, and Appendix C should be consulted for guidance in altering their values.

(**) Variables indexed from 41-50 deal with cattle-related information. They are based on information reported or developed in Small². Variables indexed from 56 to 58 and from 61 to 68 are for specific soil properties. Those suffixed '1' are associated with surface soil conditions. Those suffixed '2' are associated with sediment conditions, such as at the bottom of small lakes. Those suffixed '3' are associated with soil surrounding basements, which due to construction practices may be intermediate in properties between surface soil and sub-surface soil. Variables indexed from 76 to 84 are involved in diffusion models of vapor flux generation from contaminated soils.

(**) The variable at index 59, f(S1), appears in equations for soil pathway 1 (drinking water) and 14 (dermal exposure). The variable at index 60, f(S2),

is in the fish consumption pathway equation. They can be considered as model adjustments relative to a worst case model situation, that of water in equilibrium with the contaminated soil mass of concern. The equilibrium is described by a "Kd" (see index 118 and 119 in Table 1), which can be construed as the mg/kg of pollutant in soil required to provide 1 mg/L pollutant in water at equilibrium. At equilibrium conditions, f(S1) and f(S2) would be unity. A model (such as groundwater migration from a contaminated soil mass or overland run-off) can provide a result expressed in the same manner as a Kd, the mg/kg of pollutant in soil required to provide 1 mg/kg in water. The variables f(S1) and f(S2) are then the division of the model result respectively by Kd1 or Kd2. For example, if Kd1 was 3 mg/kg per mg/L, and a model result was 100 mg/kg per mg/L, f(S1) would be 3/100 or 0.033.

4.6.3 (**) Viewing .LDS Files

The data developed or down-loaded in INPUTS11 can be reviewed in the OPEN11 module in one of two ways. The contents are displayed on the monitor if option '3' is selected at the "DISPLAY-PRINT UTILITY MENU". The display of data in DEFALVA.LDS by this option appears in Figure 7. In this display, items 1-5 appear in the first row, 6-10 in the second row, etc. Thus, the value "6.6" at the row "40+" and column "four" is Upm (item 44 from Table 1). The contents can be printed if option '5' is selected. In this case, the identification of each variable is listed along with the datum value.

```

***** DISPLAY-PRINT UTILITY MENU *****
Input number for desired printout
Select '1' for pathway status
Select '2' for data use status table (DUST)
Select '3' for values of non-chemical data from .LDS file
Select '4' for values of chemical data from .DAT file
Select '5' for printout of variables from .LDS and .DAT files
          with narrative identities supplied.
Select '6' to quit this utility and return to main menu.

? 3
line      one      two      three      four      five
0 +       70       12       1.6       .0065     .017
5 +       .1       .3       7.400001E-05 .00018    1.5
10 +      17       1.8       1         0         0
15 +      0       0         0         0         0
20 +      0       0         1         1         1
25 +      1       1         1         1         1
30 +      1       0         1         0         0
35 +      0       0         0         0         0
40 +      .25     .04       15.3      6.6      .35
45 +      78     16.6      .87       250     520
50 +      0       0         0         0         0
55 +      .02     1.4       .1         1         1
60 +      .1     1.4       .4         .25     .001
65 +      1.6     .2        .2         0         0
70 +      0       0         0         0         0
75 +      1.34    .083      2         20        60
80 +      25000   100       .01        1         0
85 +      0       0         0         0         0

For location, read down side for multiple of 5, then across.
Last down-loaded file was ...\\themod11\\diskb\\defalva.lds. Data stored in ...
if blank, data are only accessed on-line.
Hit enter (return) to continue....

```

Figure 7. Data in DEFALVA.LDS

4.7 CHMFIL11

4.7.1 Running CHMFIL11

CHMFIL11 is accessed from OPEN11 by responding '5' to the Selection Menu (see Figure 4). Since the operations in this module are quite similar to INPUTS11, this discussion skims over common points and highlights differences.

You choose one of three options at the "MAJOR MODE OF OPERATION MENU" to process on-line information, to process a stored .DAT file in a "load and go" mode, or to modify a stored .DAT file. The review and selection (if needed) of a .DAT file parallels those of INPUTS11 for .LDS files. At the "DATA USE STATUS TABLE (DUST) LOADING PROCESS MENU", you have three options: use the on-line stored DUST (option "1"), download a DUST from a .PTH file in off-line storage (option "2"), or review all data elements (option "3").

The "DATA REVIEW AND MODIFICATION ROUTINES" follows. The module displays, one at a time, names of the variables, their status in the scenario analysis and their current values. Here, you have three options for data assessment. Option '1' accepts the value given. Only when this option is selected does the module move on to the next name and value combination. Option '2' allows you to insert a different value, and after it is selected, you are prompted for the replacement value. Figure 8 shows a portion of the display for hypothetical processing of two variables from the default file DEFALC.DAT. The display illustrates both of these responses. Option '3' transfers execution to the CHMPRP11 module where you can estimate some of the inputs which directly enter into PHAS equations. As noted in Figure 8, an advisory message is displayed indicating whether an estimation routine is available in CHMPRP11. After a routine in CHMPRP11 computes an estimated value, the estimate is presented for acceptance.

At the conclusion of the data processing routine, the chemical name listed is displayed, and you are given the option to change the name. You can input up to 255 characters (3 lines) at this prompt. Finally, CHMFIL11 displays the "STORAGE DISPOSITION MENU", whose options are the same as those in INPUTS11: no off-line storage, store data in a file with the same name as the downloaded file (modify a file), or store data in a file with a new name (create a new file). Then, control passes back to OPEN11.

4.7.2 .DAT Files

The default file DEFALC.DAT is supplied on Disk 2. Don't delete this file. Although DEFALC.DAT is not write-protected, inexperienced users should not modify this file.

(**) The variables indexed from 91 to 140 in Table 1 are stored in a .DAT file. Items indexed from 91 to 106 do not appear in pathway equations, but they can be used to estimate variables which do. These variables have been ordered so that the most fundamental variables appear first. A DUST filters out variables that are definitely not required in a PPLV analysis. For example, if you know Kwp (the water to forage partition coefficient) or plan to estimate it from log Kow, you will not need to process Ksv,

```

*****
Meat fat<-plant p.c., kg dwb forage/kg adipose tissue [Kpat] =
1.822803E-03
Status in scenario is:Item may be needed to estimate input variable

Select '1' to accept value.
Select '2' to insert new value.
Select '3' to enter estimation routine for value
Estimation routine available.

Enter your selection: 1
*****
Fish bioconcentration factor, L/kg fish [BCF] = 10.15409
Status in scenario is:Main input variable

Select '1' to accept value.
Select '2' to insert new value.
Select '3' to enter estimation routine for value
Estimation routine available.

Enter your selection: 2
Input revised value.? 13
*****
Fish bioconcentration factor, L/kg fish [BCF] = 13
Status in scenario is:Main input variable

```

Figure 8. Sample Display of Data Handling Routine in CHMFIL11

Ksp, their associated foc values, or Kwv (other variables from which Kwp could be estimated). This points up the utility of reviewing the printout from PATWAY11 (Figure 5) before doing operations in CHMFIL11.

(**) Variables indexed from 131 to 136 relate to type 1 constraints (see Section 2.0). If you are preparing a .DAT file and data are not available for such a variable, enter a negative number as the variable value. This will prevent extraneous listings in the module COMPUT11.

4.7.3 (**) Viewing .DAT Files

The variables in the .DAT file can be reviewed in the OPEN11 module in two ways. At the main selection menu, select function '6'. At the "DISPLAY-PRINT UTILITY MENU", select option '4'. A display similar to that in Figure 9 will appear. The placement scheme is similar to that discussed for Figure 7 (Section 4.6.3). Note that item 135 (last entry on line "130+") is assigned the value -1, a negative number to indicate no available data as noted above. You also can get a print-out of the variables by selecting option '5'; the printout includes the variable names as well as values.

4.7.4 Pre-packed Files

PHAS includes prepared .DAT files for Army explosive-related substances. Each .DAT file has a corresponding .DOC file, where documentation for the data in the .DAT file appears. The .DOC files are in text format, and can be reviewed with conventional word-processing programs (the files were prepared with WordStar 2000). Users should review the .DOC file for special advisories concerning variable defaults. Variables which may require re-calculation prior to use in COMPUT11 are Kpm, Kpd, Kd1, Kd2, and Kd3. In some situations, their recalculation requires data in an .LDS file (such as


```

***** DISPLAY-PRINT UTILITY MENU *****
Input number for desired printout
Select '1' for pathway status
Select '2' for data use status table (DUST)
Select '3' for values of non-chemical data from .LDS file
Select '4' for values of chemical data from .DAT file
Select '5' for printout of variables from .LDS and .DAT files
        with narrative identities supplied.
Select '6' to quit this utility and return to main menu.

? 4
line      one          two          three          four          five
90 +      227          150          291.8719        2.34          .3
95 +      .01          0          0          0          0
100 +     1000          1.3          1.605018        .02          .02
105 +     1.822803E-03  0          0          0          0
110 +     10.16409      32.10037      35          4.657008E-04  7.291213E-05
115 +     1.220268E-02  .55          20          50          3
120 +     .0008         0          0          0          0
125 +     .001          .01          0          0          0
130 +     50           .15          .01          100         -1
135 +     .02           0          0          0          0
Data is for substance Trinitroanything
For location, read down side for multiple of 5, then across.
Last down-loaded file was ...\\themod1\\diskb\\defalc.dat . Data stored in ...
If blank, data are only accessed on-line.
Hit enter (return) to continue....

```

Figure 9. Data in DEFALC.DAT

fraction organic carbon or fraction fat in meat). These recalculations may be carried out in CHMPRP11 by access through CHMFIL11. Moreover, some specific "global" calculations can be carried out more quickly in COMPUT11, and the reader should consult Section 4.8 for details.

4.8 COMPUT11

COMPUT11 is accessed from OPEN11 by responding '7' to the Main Function Selection Menu (see Figure 4). The module starts with three similarly-written routines to identify the source of the DUST, non-chemical data, and chemical data, and to transfer these data into COMPUT11. First, if a set of data are stored on-line, you have the option to use that set. You are prompted:

```

Enter 'yes' or 'no'
Do you want on-line (pathway) (non-chem input) (chemical input) data?

```

Respond 'yes' to use the on-line data set. A response of 'no' will cause a prompt: "Do you want to see (.PTH) (.LDS) (.DAT) files?" A 'yes' response to this query is followed by a display of the available files. Next, you are prompted to enter a filename. After the designated file is down-loaded, and the three sequences are completed, the next display is:

```

***** HUMAN TARGET SELECTION *****
Input '1' is an adult target is to be selected
Input '2' if a child target is to be selected.

```

Select '1' or '2' as appropriate. This selection governs whether the product $BW \times D_T$ or $BW_c \times D_T$ is the limiting intake that determines the PPLV (see equation 3 in Section 2.0). Following this display, if you are doing a soil PPLV analysis, there are two computation option selections. The first is to set $Kd_i = Koc \times foc_i$, where Koc and the foc_i ($i = 1, 2$ or 3) are from on-line data. After the prompt display, enter '1,' to do this, otherwise, enter '2'. If you enter '2,' the values of Kd_1 , Kd_2 , and Kd_3 currently on-line will be used. The next option is to compute Kpm and Kpd from $Kpat$ using the relations $Kpm = Kpat \times fm$ and $Kpd = Kpat \times fd$ where $Kpat$, fm , and fd are supplied from on-line data. Procedures follow those described above for Kd .

The module next computes the input equations shown in Appendix B and presents the results in terms of environmental medium limits (corresponding to SPLV and PPLVs) as well as intakes. The display showing the analysis of the scenario of file S036AC.PTH (the sample problem from Section 4.4) with the down-loaded data from the files DEFALVA.LDS and DEFALC.DAT appears in Figure 10.

Three sets of results are displayed. The "UNIT INTAKE" column indicates the mg/day intake of pollutant via each specific pathway resulting from 1 mg/L in water or 1 mg/kg in soil. These values are the R_i discussed in Section 2.0. The next column shows the SPLVs, as defined by equation 4 in Section 2.0. The final column, "PPLV INTAKE", is the mg/day of pollutant intake corresponding to a PPLV concentration in water or soil. The sum of intakes in this column is the "ALLOWABLE DAILY INTAKE", $BW \times D_T$ or $BW_c \times D_{TC}$. The PPLV is computed from equation 5 of Section 2.0.

Next, the module displays an informative "CONSTRAINT ANALYSIS" description and prompts for a response from 0 to 3. The entry '0' will cause control to pass back to OPEN11. The entry '1' or '3' causes the Type 1 constraint analysis routine to be executed. This routine tests whether the pollutant concentration indicated by the PPLV could be harmful in other respects. Based on the pathway chosen, these effects can include:

- * Organoleptic effects (color, unpleasant taste or odor) in water.
- * Undesirable effects, such as death, reduced reproduction or toxic effects to aquatic biota species.
- * Phytotoxic impact on commercially important plants.
- * Adverse economic impact or health effects to livestock or dairy cattle.

As the selected pathways are analyzed, a message will be displayed indicating the constraint-limiting concentration followed by the message:

PPLV OK FOR (specific situation)
or the message:
Potential constraint: (adverse effect).

Pauses are inserted to allow you to print hard copy. Figure 11 shows a portion of the analysis for the sample problem. Here, livestock effects

```

***** HUMAN TARGET SELECTION *****
      Input '1' if an adult target is to be selected
      Input '2' if a child target is to be selected. Input: 1
***** OPTION TO COMPUTE KD = KOC x FOC *****
      This option is recommended for pre-packed .DAT files where the
      above equation is a reasonable representation of soil sorption.
      Input '1' for the option, '2' to continue (existing KD values
      will be used). 2
***** OPTION TO COMPUTE Kpm AND Kpd FROM fm AND fd *****
      This option is recommended for pre-packed .DAT files where the
      chemical conc. is expected to depend on fat content. The part.
      coefficients are  $K_{pm} = K_{pat} \times f_m$  and  $K_{pd} = K_{pat} \times f_d$ .
      Input '1' for the option, '2' to continue with existing on-line
      values. 2

***** PPLV COMPUTATIONS *****
      SUBSTANCE NAME IS Trinitroanything

      PATH                UNIT INTAKE          SPLV          PPLV INTAKE
                        mg/day per             mg/kg          mg/day at PPLV
                        mg/kg
      Eat Vegetables      2.719E-02            2.575E+00        5.629E-02
      Eat Beef [P+S+W]    8.398E-05            8.335E+02        1.739E-04
      Norm. Soil/Dust     7.400E-05            9.459E+02        1.632E-04
      Diffusing vapor/inside 6.463E-03            1.083E+01        1.338E-02

      PPLV IS 2.070E+00                                mg/kg

      ALLOWABLE DAILY INTAKE IS .07 mg/day
      Hit enter (return) to continue....

```

Figure 10. PPLV Analysis for Sample Problem

may pose a potential constraint, since the PPLV of 2.07 mg/kg is ten times higher than the computed "critical concentration" of 0.206 mg/kg.

The type 2 constraint analysis occurs either at the end of a type 1 constraint analysis when option '3' is selected or when option '2' is selected. It is announced by the line:

***** TYPE 2 CONSTRAINT ANALYSIS *****

The analysis continues automatically. If the medium selected is water, the analysis returns one of two messages:

PPLV not subject to Type 2 constraint
or

PPLV exceeds solubility limit. Type 2 constraint exists.
Criteria levels in excess of the PPLV may be justified.

The module returns control to OPEN11. If the medium selected is soil, each pathway in the scenario is tested, and a status message is displayed:

Path (description) type 2 constraint status = (yes or no)

An example appears in Figure 12, which is for the sample problem. After the tests, one of two summary messages will be displayed:

You can choose one of four options. Enter '0' to do no analyses.
Enter '1' to do ONLY a Type 1 analysis. Enter '2' for ONLY a Type 2
analysis. Enter '3' to do BOTH analyses.

Enter your selection here: 3

***** CONSTRAINT ANALYSIS *****

TYPE 1 CONSTRAINT. For reference, PPLV = 2.070448 mg/kg

Test for soil pathway # 3 Eat Vegetables

TEST based on Phytotoxic limit in hydroponic solution, mg/L

CRITICAL CONC. = 2007.143 mg/kg

PPLV OK FOR PLANTS(based on water data)

Hit enter (return) to continue....

Test for soil pathway # 6 Eat Beef [P+S+W]

TEST based on Acceptable limit dose to cattle, mg/kg-day

CRITICAL CONC. = .2055387 mg/kg

POTENTIAL CONSTRAINT:livestock adverse effects

Hit enter (return) to continue....

TEST based on Phytotoxic limit in hydroponic solution, mg/L

CRITICAL CONC. = 2007.143 mg/kg

PPLV OK FOR PLANTS(based on water data)

Hit enter (return) to continue....

No Type 1 constraints for soil pathway # 10 Norm. Soil/Dust

No Type 1 constraints for soil pathway # 10 Norm. Soil/Dust

No Type 1 constraints for soil pathway # 10 Norm. Soil/Dust

No Type 1 constraints for soil pathway # 12 Diffusing vapor/inside

No Type 1 constraints for soil pathway # 12 Diffusing vapor/inside

No Type 1 constraints for soil pathway # 12 Diffusing vapor/inside

*****NOTE***** If no test messages were displayed concerning

Type 1 Constraint, no soil pathways other than pathways 10

through 13 were included in the scenario.

End Type 1 Constraint Analysis

Hit enter (return) to continue....

Figure 11. Part of the Type 1 Constraint Analysis, Sample Problem

Type 2 constraint flagged, PPLV adjustment attempted.

or

Solubility will not pose a type 2 constraint.

In the latter case, control transfers to OPEN11. If there is a Type 2 constraint, a routine is automatically executed to compute a soil limit higher than the PPLV which meets the consumption constraint used to compute the PPLV (for more details, see Small² or Section A.7.3 in Appendix A).

If no PPLV adjustment can be done, the message "PPLV may not be applicable. System totally constrained." will appear, and control is returned to OPEN11. If there is an adjustment, the message "Adjusted PPLV is (number) mg/kg." will appear. Since a higher soil limit may trigger additional type 2 constraints, this procedure is repeated until no further upwards adjustment of the PPLV can occur. At this point, the message "No further adjustment needed. Analysis over." will appear. The module then returns control to OPEN11.

At the conclusion of a COMPUT11 session, the information used in the analysis will be in on-line storage. It can be viewed in OPEN11 (see Sections 4.5.3, 4.6.3, and 4.7.3). You can go to CHMFIL11 or INPUTS11 to modify chemical or non-chemical data for "what-if" type analyses. If you had entered '1' for either the "OPTION TO COMPUTE KD = KOC x FOC" or the "OPTION TO COMPUTE K_{oc} AND K_{od} FROM f_{oc} AND f_{od}", the values computed by the selected options will be placed in on-line storage, replacing those that were in on-line storage at the start of COMPUT11 execution.

```

***** TYPE 2 CONSTRAINT ANALYSIS *****

For reference, Water solubility, mg/L [SW] = .3
PPLV = 2.070448
Path Eat Vegetables type 2 constraint status = no
Path Eat Beef [P+S+W] type 2 constraint status = no
Path Norm. Soil/Dust type 2 constraint status = no
Path Diffusing vapor/inside type 2 constraint status = yes
Path type 2 constraint status = no
Path type 2 constraint status = no
Path type 2 constraint status = no
*****NOTE*****Expect non-defined pathways if pathways 5 or 6 or 8 or 9
were in scenario.
Hit enter (return) to continue....

Type 2 constraint flagged, PPLV adjustment attempted
Adjusted PPLV is 2.338205 mg/kg.
Now checking to see if further adjustment is needed
Path Eat Vegetables type 2 constraint status = no
Path Eat Beef [P+S+W] type 2 constraint status = no
Path Norm. Soil/Dust type 2 constraint status = no
Path Diffusing vapor/inside type 2 constraint status = yes
Path type 2 constraint status = no
Path type 2 constraint status = no
Path type 2 constraint status = no
*****NOTE*****Expect non-defined pathways if pathways 5 or 6 or 8 or 9
were in scenario.
Hit enter (return) to continue....

Type 2 constraint flagged, PPLV adjustment attempted
Adjusted PPLV is 2.338205 mg/kg.
Now checking to see if further adjustment is needed
No further adjustment needed. Analysis over.
READY TO RETURN TO OPEN11
Hit enter (return) to continue....

```

Figure 12. The Type 2 Constraint Analysis for the Sample Problem

4.9 The Sample Problem

The sample problem was stated in Section 4.4. The compound "trinitroanything" was in soil at a site at concentrations as high as 2 mg/kg. The existing life-style scenario was processed in PATWAY11 and stored in the file S036AC.PTH (Figures 5 and 6). Intake and area conditions were expressed by the data in DEFALVA.LDS (Figure 7). Specific information for "trinitroanything" was in the file DEFALC.DAT (Figure 9).

The PPLV analysis (Figure 10) indicated that, based on an allowable intake of 0.07 mg/day (the D_T of "trinitroanything" is 0.001 mg/kg-day; the target human weighs 70 kg), the PPLV is 2.07 mg/kg. However, the Type 2 constraint analysis indicates this may be conservative, since water solubility limits the contribution that the soil-diffusion pathway can make to "trinitroanything" intake. Adjusting for this limitation, the 0.07 mg/day intake would be attained with a soil level of 2.34 mg/kg. However, cattle may experience adverse effects at a 0.21 mg/kg soil level (Figure 11). Since cattle have been exposed to "trinitroanything" at the site for some time, as a minimum, the adverse health effects or economic impacts to animals at the site should be addressed. If the constraint analysis predictions are validated, some type of remedial action would be warranted.

5.0 CHMPRP11

The CHMPRP11 module in PHAS has 24 subroutines, of which 14 contain both information messages and estimation methods. The other 10 contain only information messages. CHMPRP11 can be accessed from CHMFIL11 (see section 4.7.1) or from OPEN11 on an "a la carte" basis. Section 5.1 describes the interfaces between CHMPRP11 and CHMFIL11 or OPEN11, while Section 5.2 describes specific estimation subroutines. The selection of CHMPRP11 estimation methods was based upon wide applicability and minimal input requirements. Many have been adapted from Lyman et al.⁶, which can be consulted for other estimation methods.

5.1 Running CHMPRP11

CHMPRP11 is accessed either directly from OPEN11 by entering '9' when prompted by the "MAIN FUNCTION SELECTION MENU" or from CHMFIL11 by entering '3' when prompted in CHMFIL11's "DATA REVIEW AND MODIFICATION ROUTINES".

The initial CHMPRP11 displays differ, depending on the accession mode. When it is accessed from OPEN11, the selection menu display (Figure 13) appears. The property subroutine desired is selected by entering the specified designation number. Subroutine selections marked with an asterisk only provide a descriptive information message (for example, see "Mol Weight" in Figure 13). In the execution of any subroutine, an information message is first displayed. After you exit an description-only subroutine, you encounter the exit prompt:

```
Answer 'yes' or 'no'
Wish to Do More?
```

A 'yes' response sends you back to the selection menu shown in Figure 13, a 'no' response sends you back to OPEN11. In subroutine with an estimation method, the information message is followed by a method selection menu. Most data inputs are manual. At the conclusion of the selections and the display of results, the above exit prompt is encountered. If you answer 'yes', you return to the selection menu shown in Figure 13; if you answer 'no', you exit back to OPEN11.

When CHMPRP11 is called from CHMFIL11, the CHMPRP11 subroutine corresponding to the variable being processed is accessed; Figure 13 is not displayed. In most estimation method subroutines, the data in on-line storage is accessed, so manual data inputs are minimal. At the end of each subroutine, you encounter the exit prompt shown above. However, a 'yes' input sends you back to the subroutine's information message. This feature is useful if you wish to see the estimates provided by different methods. With a 'no' response, control reverts back to CHMFIL11.

The order of CHMPRP11 subroutines presented in Figure 13 is based on a hierarchy of information needs. Thus, the subroutines dealing with molecular weight and log Kow precede those for which their use is required. Keep this in mind when deciding which calculation routines to attempt. In estimation

***** WELCOME TO THE CHEMICAL PROPERTIES ESTIMATION MODULE *****

***** HERE IS A LISTING OF PROPERTIES ESTIMATED *****

Check your user's guide since you may need a property in the estimation process which must be first estimated.

1 = Mol Weight(*)	2 = Melting point(*)	3 = Boiling point
4 = Log Kow(*)	5 = Water solubility	6 = Sat. vapor pressure
10 = Koc	11 = Ksp(soil/plant)	12 = Ksv(soil/veg)
13 = Reference focs for Ksp and Ksv(*)		
15 = BCF for fish	16 = Kwv(water/veg)	17 = Kwp(soil/plant)
18 = Kpat (fat/plant)		19 = Kpm(plant/meat)
20 = Kpd (plant/milk)		21 = Kh (Henry Law)
22 = Da (air diffusivity)		23 = Kd (soil/water)
24 = Dermal permeability(*)		25 = DT(*)
26 = DTc(*)		27 = Organolept. limit(*)
28 = Aquatic tox limit(*)		29 = Cattle tox limit
30 = Phytotoxicity limit(*)		31 = Exit to OPEN11 now

An asterisk (*) indicates a VERBAL description only, no calculations.

Input the number of your selection:

Figure 13. Selection Menu Display of CHMPRP11

method subroutines, the data input requirements are displayed. You have the option not to do a calculation; this is useful if you wish to review the methods or find that your input data base is not complete. In that case, you are returned to the exit prompt. Each calculation option prompts you for data. These options are described in Section 5.2. Each computation concludes with a display of input data and the result.

The subroutines for Kpm and Kpd (see Sections 5.2.9 and 5.2.10) have estimation methods requiring use of the site-specific variables fat fractions in beef and dairy (fm and fd). The estimation methods for Kd (see Section 5.2.13) require site-specific fraction of soil organic carbon (foc) data. Options are provided to obtain these data from a .LDS file. If a .LDS file is down-loaded in CHMPRP11, regardless of whether entry was from CHMFIL11 or OPEN11, its contents stay in on-line storage until another .LDS file is down-loaded.

5.2 CHMPRP11 Estimation Subroutines

5.2.1 Boiling Point

Two methods are presented. The first is an inverse form of the Lorenz and Herz correlation to predict the melting point from the boiling point, which was presented by Gold and Ogle⁷. It is not recommended for aldehydes, alcohols, and polar hydrocarbons. The second method, developed by Miller, is discussed in Section 12-5 of Lyman et al.⁶. It requires knowledge of a substance's structure in terms of the specific fragments indicated in Figure 14. Figure 14 also shows the fragments presentation tableau (both the instructions and tableau are displayed in CHMPRP11). This tableau follows the order of Table 12-12 in Lyman et al.⁶.

The CRT will display 41 different structure fragments in a table. You will be prompted to enter the identification number for a given fragment (FIN) of the subject pollutant and then the number of times that fragment occurs in the pollutant molecule. Your entry will be echoed back. You will be queried if you wish to do more. If you select yes, the table will re-display with the previous selection posted. This sequence is repeated until you respond 'no' to the 'Do you want to do more?' query.

In the table, there are coded abbreviations. 'NR' indicates a non-ring structure, 'RG' a ring. Rings can be either aliphatic or aromatic. Other abbreviations are alc=alcohol, phi=phenol, ald=aldehyde, est=ester. The triple bond (see FIN9 and FIN10) appears as '-#'. As examples of input, dinitrophenol would appear as 3FIN14 (=CH- in a ring), 3FIN16 (=C< in a ring) 1FIN22 (phenolic OH), and 2FIN37 (nitro groups). The compound DBCP 1,2-dibromo-3-chloropropane or CH2Br-CHBr-CH2Cl appear as 2FIN2 (-CH2- non-ring), 1FIN3 (-CH< non-ring), 2FIN19 (bromine), and 1FIN18 (chlorine). Entries need not be made in FIN order.

Enter 'yes' or 'no'.
Do you wish to continue analysis? yes

MILLER BOILING POINT METHOD FRAGMENTS ID TABLE

OFIN1 -CH3 [NR]	OFIN2 -CH2-[NR]	OFIN3 -CH< [NR]	OFIN4 >C< [NR]
OFIN5 =CH2 [NR]	OFIN6 =CH- [NR]	OFIN7 =C< [NR]	OFIN8 =C= [NR]
OFIN9 -#CH [NR]	OFIN10 -#C- [NR]	OFIN11 -CH2- [RG]	OFIN12 -CH< [RG]
OFIN13 >C< [RG]	OFIN14 =CH- [RG]	OFIN15 =C< [RG]	OFIN16 =C= [RG]
OFIN17 -F	OFIN18 -Cl	OFIN19 -Br	OFIN20 -I
OFIN21 -OH alc	OFIN22 -OH phi	OFIN23 -O- [NR]	OFIN24 -O- [RG]
OFIN25 >C=O [NG]	OFIN26 >C=O [RG]	OFIN27 -CH=O ald	OFIN28 -COOH acid
OFIN29 -COO- est	OFIN30 =O other	OFIN31 -NH2	OFIN32 >NH [NR]
OFIN33 >NH [RG]	OFIN34 >N- [NR]	OFIN35 >N- [RG]	OFIN36 -CN
OFIN37 -NO2	OFIN38 -SH	OFIN39 -S- [NR]	OFIN40 -S- [RG]
OFIN41 =S			

When prompted, enter FIN. Enter number of units next
Enter FIN (from 1 to 41) here: 2

Enter number of specified fragments in molecule. 6

Figure 14. Miller Boiling Point Method Displays: Information and Tableau.

The subroutine prompts for a fragment identifier number (FIN) and the number of times the identified fragment occurs in the pollutant molecule. After entry of these data, the tableau display is revised to show the input. After this "roll-over", the message "Do you want to do more?" is displayed. Until there is a 'no' response, the subroutine continues to query for a FIN and the number of fragments. You continue making entries until you are through (you can also correct errors, and replace a non-zero value with zero). The routine determines and displays the molecular weight from your inputs. If you entered CHMPRP11 from CHMFIL11, the molecular weight in on-line storage is also displayed. If considerable error exists between them (other than round-off errors; in routine computations, weights are to the nearest 0.1 units), either the tableau entries or the molecular weight in the on-line data set are incorrect.

5.2.2 Water Solubility

Four equations are included in this subroutine. If you enter CHMPRP11 from CHMFIL11, the only inputs requested are equation selections. The equations are octanol-water partition coefficient-based correlations, and have been presented in Lyman et al.⁶. Equations 2.2 and 2.15 from Lyman et al.⁶

compute a molar water solubility, thus molecular weight data is required to convert to a mg/L basis. Equation 2.15 is presented in two formats; one includes a melting point correction term, which is claimed to be somewhat more accurate for substances that are solids above 25 °C⁶. If you choose this option, you are prompted for a melting point in °C. If you enter a melting point below 25°C, the input is ignored.

5.2.3 Vapor Pressure

Five computation options are provided for vapor pressure; they are summarized in an information message (Figure 15). Before you select an option, you are queried:

Enter temperature in DegC for calculation result:

Enter the temperature applicable to the PPLV analysis (usually 25 °C). The options are discussed below. Where vapor pressure inputs are required, they are understood to be in mm Hg or torr.

Mackay's method #1. This was presented in Mallon, et al⁸. If CHMPRP11 is entered from OPEN11, you are queried for melting point and boiling point in °C. The answer is then displayed. If you enter CHMPRP11 from CHMFIL11, the on-line melting point and boiling point data are accessed, and the answer displayed.

Watson's boiling point method. This is described in Lyman et al.⁶, sections 14-3 and 14-4. If CHMPRP11 is entered from OPEN11, you are queried for boiling point in °C. Then you are queried for the substance's physical state at the calculation temperature:

Is substance a liquid at calculation temp?

Respond "yes" for a liquid, "no" for a solid. A message followed by a list identifying types of compounds is displayed (Figure 16). From this list, you select the identification number for the type of compound that best describes the substance considered. A value of K_f^* corresponding to the identification number is used to evaluate equation 14-16 from Lyman et al.⁶ The result display shows the boiling point, the state of the substance, and the vapor pressure.

If entry is from CHMFIL11, the on-line stored boiling point is accessed, and the program automatically determines whether the substance is solid or liquid. Here, the first query by the subroutine is the identification number from Figure 16. Execution follows as noted above.

Simple interpolation. This is based on the Clausius-Clapeyron equation, which states that, within a short range of temperature, $\log P \propto T^{-1}$, where T is in degrees Kelvin. The subroutine requests two sets of temperatures and pressures are requested, first for the lower end of the range, and next for

* The K_f values are in Lyman et al.⁶ Table 14-4. The values used here correspond to the six-carbon column in that table.

```

***** VAPOR PRESSURE METHOD SELECTION MENU *****
Select '0' to exit without estimation
Select '1' for Mackay's Method e1 for both liquid and solids. If you're
here from OPEN11, you must input Tmelt and Tboil.
Select '2' for Watson's boiling point method for both liquids and solids.
If you're here from OPEN11, you must input the liquid boiling point and
the state of the substance (liquid or solid) at ambient conditions.
Select '3' for simple interpolation. You enter two data pair sets of
saturation vapor pressure/ temperature. The sets must be for either
the solid or liquid state, but not one of each. If you're here from
OPEN11, and your data pair sets are for the liquid state, but you want
a solid state VP, you will be prompted for Tmelt. You can't estimate
a liquid-state VP by this method from solid state data.
Select '4' for Mackay's Method modified for input of only the melting point.
Tboil is approximated internally. This is the least accurate of the
methods. No additional inputs are needed if you're here from CHMFIL11.
Select '5' for Watson's reduced pressure method. This is similar to
selection '2' above but uses a paired reduced pressure and temperature
input in place of the boiling point.
Enter your selection (from 0 to 5):

```

Figure 15. Vapor Pressure Estimation Method Selection Menu.

```

Enter temperature in DegC for calculation result: 27
Enter boiling point in DegC: 444
Enter 'yes' or 'no'.
Is substance a liquid at calculation temp? yes
You will be shown a table of general compound groups. Choose the
number of the structure best describing your compound. For mixed
aromatic constituents, -OH takes precedence. For simple aromatics
consider the phenyl group as a n-Alkane (selection e1).
Press enter (return) key to continue....

```

```

***** TABLE OF STRUCTURE IDENTIFICATION FACTORS FOR VP ESTIMATIONS *****
***** Aliphatic and Carbocyclic/ Heterocyclic Cmps. with Aliphatic Props.
1. n-Alkanes                2. Other alkanes                3. Olefins
4. Cyclic sat. hydrocarbs  5. Alkylated cyclic sat. hydrocarbs
6. Monochloride             7. Monobromide                 8. Moniodide
9. Polyhalide (not entirely halogenated) 10. Totally halogenated cpd.
11. Perfluorocarbon         12. Ester (R-COO-R')          13. Ketone
14. Aldehyde                15. Primary amine             16. Secondary amine
17. Tertiary amine          18. Nitrile                   19. Nitro compound
20. Mercaptans              21. Sulfides
22. Alcohol(single OH)      23. Diols                     24. Triols
25. Cyclohexanol, cyclohexyl methyl alcohol, etc.
26. Aliphatic ethers        27. Oxides (cyclic ethers)
***** Aromatic Compounds (use phenol values if mixed function on ring)
27. Monophenols             28. Other phenols(2 or more -OH)
29. Monoaniline             30. Other aniline(2 or more -NH2)
31. N-sub. anilines (C6H5NHR) 32. Naphthols (one -OH)
33. Naphthylamines (one -NH2) 34. N-Substitued naphthylamines
35. ANY OTHER COMPOUND(Default value)
Enter identification number:

```

Figure 16. Watson Boiling Point Structure Display.

the upper end of the range. The routine next queries:

Enter '1' if substance is liquid at calc. temp & in range.

Enter '2' if substance is solid at calc. temp but liquid in range.

Enter '3' if substance is solid at calc. temp & in range.

Provide the entry for your compound and calculation temperature situation. The vapor pressure is computed directly if '1' or '3' is your response. If your response is '2', you are queried for a melting point in °C. In this case, the vapor pressure initially computed is that of a "supercooled liquid". This is converted to a solid vapor pressure by equation 14-10 of Lyman et al.⁶. This method is most accurate when the calculation temperature is inside the range. In case of an extrapolation of more than about 25 °C outside of the range, Watson's reduced pressure method (see below) may be more accurate, and only requires one data set.

Mackay's method (modified). This method uses the Lorenz and Herz equation (see Section 5.2.1) to estimate the boiling point from the melting point. Then, the melting point and estimated boiling point are entered into Mackay's Method #1. You are prompted to enter the melting point if entry is from OPEN11; otherwise, the melting point in on-line storage is accessed.

Watson's reduced pressure method. This routine is based on equations 14-24 and 14-26 in Lyman et al.⁶. However, in place of the boiling point at 1 atmosphere pressure, a paired set of vapor pressure-temperature data are entered. Generally, the vapor pressure used is below 1 atmosphere, hence the name "reduced pressure". You supply the reference temperature and pressure at the prompts:

Enter reference temperature for reduced pressure:

Enter VP at reference temperature:

If you entered CHMPRP11 from OPEN11, you are asked "Is substance a liquid at calculation state?" to which you provide a "yes" (for liquid) or "no" (for solid) response. The the display in Figure 16 appears next, and after you select the identification number, the conditions of the problem and estimated vapor pressure are displayed.

5.2.4 Koc

This subroutine provides 7 different correlation equations; they are identified in the system display shown in Figure 17. If you enter CHMPRP11 from OPEN11, you are queried to supply the requisite data, after which the estimated Koc is displayed. If you enter CHMPRP11 from CHMFIL11, no inputs are required after selection of the correlation equation.

5.2.5 Ksp and Ksv

Although each variable has a separate entry value when CHMPRP11 is entered from OPEN11, one subroutine processes both of them. One estimation method is used, which was proposed by Travis and Arms⁹ for "vegetation":

***** INFORMATION ON *****
 Soil organic carbon to water partition coefficient, L water/kg OC [Koc]

Koc is the ratio between the equilibrium pollutant concentration on soil organic carbon (SOC) and the concentration in water. Koc indicates the relative distribution of pollutant between soil and water assuming that pollutant in soil is primarily physically adsorbed on SOC. Kd can be estimated from Koc: $K_d = f_{oc} \times K_{oc}$ where f_{oc} is the fraction of SOC in soil. Kd is an input to many SPLV equations and to constraint tests where water-based data are used for comparison to soil results.

Seven methods are presented here. The first six were presented in the Final Report, Task 16, EPA Contract 68-01-6951. The 7th is equation 4-5 in Lyman, et. al. Chemical Property Estimation Methods.

Select '0' to exit without calculation
 Select '1' for Lyman-Loreti (L/L) general eqtn (needs Log Kow)
 Select '2' for L/L non-aromatic eqtn (needs Log Kow)
 Select '3' for L/L aromatic eqtn (needs Log Kow)
 Select '4' for L/L general eqtn (needs Mol Wt, mg/L solubility)
 Select '5' for L/L non-aromatic eqtn (needs Mol Wt, mg/L solubility)
 Select '6' for L/L aromatic eqtn (needs Mol Wt, mg/L solubility)
 Select '7' for Kenaga eqtn (needs mg/L solubility)
 Enter your selection (from 0 to 7):

Figure 17. Koc Estimation Method Selection Menu

$$\log K_{sp} = 1.588 - 0.578 \times \log K_{ow}$$

If you entered CHMPRP11 from OPEN11, you are prompted to enter a value of log Kow ; otherwise, no input is required.

5.2.6 BCF

Three estimation options are presented, corresponding to equations 5-2, 5-3 and 5-4 in Table 5-1 of Lyman, et al.⁶. These equations respectively require an input of log Kow, water solubility or Koc, and after you select the equation option, if you enter CHMPRP11 from OPEN11, the applicable variable is requested. Otherwise, you supply no additional input.

5.2.7 Kwv and Kwp

Similar to Ksv and Ksp, these variables are handled in one subroutine. Option 1 uses the "modified" Briggs equation²:

$$K_{wv} \text{ or } K_{wp} = 5 \times (0.82 + 10^{E1}) \times 10^{E2}$$

where

$$E1 = 0.95 \times \log K_{ow} - 2.05$$

$$E2 = -0.178 \times (\log K_{ow} - 1.78)^2$$

You are prompted to enter log Kow if you enter CHMPRP11 from OPEN11. Options 2 and 3 compute either variable from a Ksp or Ksv input, respectively. If you have entered CHMPRP11 from OPEN11, Ksp or Ksv, a reference f_{oc} (that of the soil used in studies to determine Ksp or Ksv), and a Koc are requested. Option 4 only applies if you have entered CHMPRP11 from CHMFIL11, and equates Kwp to the current value of Kwv. The reverse can't be done directly in PHAS (there really is no clear-cut preference of Kwv over Kwp; this sequence selection is judgmental).

5.2.8 Kpat

Two methods are included, both from Garten and Trebalka¹⁰. If you enter CHMPRP11 from CHMFIL11, no inputs are needed other than the choice of method. Otherwise, log Kow is requested for the first selected method; water solubility is requested for the other.

5.2.9 Kpm

Six options are available for estimating Kpm. The first three options use Kpat as a starting point, and use the relation: $Kpm = Kpat \times fm$. The last three options use Kpd as a starting point, and use the relation: $Kpm = Kpd \times fm / fd$. Options 1 through 3 require Kpat input if you enter CHMPRP11 from OPEN11. Options 4 through 6 require Kpd input if you enter CHMPRP11 from OPEN11. Options 1 and 4 employ a default fm ($fm = 0.25$) and a default fd ($fd = 0.04$). Options 2 and 5 employ fm and fd information that must be down-loaded from an .LDS file; if either of these options is selected, you first review the stored .LDS files and are prompted to enter a filename. Options 3 and 6 employ on-line values of fm and fd (on-line data are available if an .LDS file has been previously down-loaded during the current session).

If you choose option 2, 3, 5 or 6, and $fd = 0$, an advisory message will indicate this situation. The selection menu is then displayed again for another option selection. If on-line data are available, the current values of fm and fd are displayed. After this, you continue processing with on-line data by responding 'yes' to the query:

Do you wish to continue with on-line info ?:

A 'no' response sends you back to the selection menu for another choice.

5.2.10 Kpd

Six options are available for estimating Kpd. They are "mirror images" of those used for Kpm, where fm and fd are switched in equations. Thus, the equations involved are: $Kpd = Kpat \times fd$ and $Kpd = Kpm \times fd / fm$. Options 1 through 3 require Kpat input if you enter CHMPRP11 from OPEN11. Options 4 through 6 require Kpm input if you enter CHMPRP11 from OPEN11. See Section 5.2.9 for fm or fd inputs for the different options.

5.2.11 Kh

Here, the dimensionless Kh is evaluated as the saturation vapor pressure divided by the water solubility, both evaluated at a given temperature. After the initial display, you are asked

Is temperature of calculation 25C (298.2K) ?

If you respond 'no,' you are prompted to enter a temperature. If you enter CHMPRP11 from CHMFIL11, there are no further inputs, and the result is displayed.

If you enter CHMPRP11 from OPEN11, you are first queried for molecular weight. Then you are queried for the units in which you plan to express water solubility data (mg/L, moles/L, or millimole/L are accepted). After this, enter the numerical value for water solubility. This sequence is repeated for the saturation vapor pressure (allowable inputs are in torr or mm Hg, atmospheres, and pascals).

5.2.12 Da

Whether you enter CHMPRP11 from OPEN11 or CHMFIL11, you are first prompted to enter the computation temperature (Tref) in degrees Centigrade. Two options are presented: an empirical method and the Fuller, Schettler and Giddings (FSG) method discussed in Section 17-4 of Lyman et al.⁶. The empirical method uses an approximation suggested by Small²

$$Da = 8 \times (Tref / 298.2)^{1.75} / (Mol\ Weight)^{0.5}$$

where Da is in m²/day, and Tref is in °K. Thus, for entry from OPEN11, you provide the molecular weight and the result is displayed.

The FSG method employs the "LeBas Volume" as input, which can be estimated from structural constituents of the substance according to Table 17-5 of Lyman et al.⁶ The instructions are shown in Figure 18, as are the atoms/structures of Table 17-5. You are prompted: Enter IDs of constituent here: When you furnish the atom/structure constituent identification number, the cursor moves to the right of the item in the tableau, where you enter the number of times the given constituent appears in the molecule. Then you are prompted (near the bottom of the screen): "Do you want to do more (respond yes or no)?" Until you respond 'no', the routine to enter information is continued. When you respond 'no', Da is computed and displayed. If the LeBas volume is below 1, you have probably left out some components of the molecule. In that case, an error message is issued, and you are sent back to the FSG method instruction message.

The routine determines and displays the molecular weight from your inputs. If you entered CHMPRP11 from CHMFIL11, the molecular weight in on-line storage will also be displayed. If there is considerable error between them (other than round-off errors; in computations, weights are to the nearest 0.1 units), either the tableau entries or the molecular weight in the on-line data set are incorrect.

5.2.13 Kd

The routine estimates Kd from the relation $Kd = foc \times Koc$. If you enter CHMPRP11 from CHMFIL11, Koc is accessed from on-line storage. However, there are three Kd numbers that may be evaluated in PHAS, and each may have a different foc associated with it. You have three options for obtaining foc :

- o down-load foc from a .LDS file (option 1)
- o use on-line foc data (option 2)
- o manual input (option 3).

Enter temperature of computation in Deg C: 25
 ***** INSTRUCTIONS FOR LE BAS VOLUME EVALUATION (FSG METHOD) *****
 The CRT will display the FSG method structure units.
 You will be prompted to enter the structural constituent
 identification number for a constituent in the pollutant.
 The cursor will move to that item. There, you enter the number
 of units in the pollutant structure. For example,
 If your structure was CH₂Cl-CHBr-COOH, you would enter:
 IDe1 [C] 3; IDe2 [H] 4; IDe4 [Br] 1; IDe6 [Cl],1 ; and ID e9
 [Carboxylic O] 2. At the end of each entry, you are queried
 to continue with entries, and the sequence above is repeated
 until you respond 'no' to this query.
 Press enter (return) key to continue....

LEBAS VOLUME CONSTITUENT UNITS			
IDE1 (C)	0	IDE2 (H)	0
IDE3 (O in Meth esters/ethers)	0	IDE4 (Br)	0
IDE5 (O in Eth ester/ethers)	0	IDE6 (Cl)	0
IDE7 (O in other esters/ethers)	0	IDE8 (F)	0
IDE9 (O in carboxylic acids)	0	IDE10 (I)	0
IDE11 (O bonded to S,P or N)	0	IDE12 (S)	0
IDE13 (other bonded O)	0	IDE14 (3 member ring)	0
IDE15 (Double bonded N)	0	IDE16 (4 member ring)	0
IDE17 (N in primary amines)	0	IDE18 (5 member ring)	0
IDE19 (N in sec. amines)	0	IDE20 (6 member ring)	0
IDE21 (Anthracene ring)	0	IDE22 (Naphthalene ring)	0

Enter IDE when prompted. Then cursor will move to IDE location.
 At that location, enter the number of units.
 Enter IDE of constituent here:

Figure 18. FSG Method Instruction and Component Tableau Display

If you select option 1, you first get a review of existing .LDS files and then are prompted to enter a file. When the information is down-loaded, you will get the message:

The fraction organic carbon (foc) used is [value]

and the computed Kd is displayed. If you select option 2, the above message and answer are also displayed. If you select option 3, you are prompted to enter foc, after which the computed Kd is displayed. When you select options 1 or 2, the program checks whether any of the on-line stored foc values are zero. If so, an error message is displayed, and you will have to either select another method or choose another .LDS file.

If you enter CHMPRP11 from OPEN11, only option 3 can be used. Thus, you are prompted to provide both Koc and foc.

5.2.14 Cattle Toxicity Limit.

This subroutine estimates a limiting dose for cattle based on extrapolation from either:

- o The long term human no observed effect dose level (NOEL)
- o A mammalian lifetime NOEL
- o A mammalian 90-day NOEL

For entry from OPEN11, you must enter the long term human NOEL; for entry from CHMFIL11, this value is on-line. For entry from OPEN11 and from CHMFIL11, you must the mammalian NOEL data for the last two of these options.

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* The Environmental Reporter and Chemical Regulation Reporter are updated frequently to include the most recent revisions to referenced material. The cited document is current to the date of this report.

APPENDIX A. SOURCE CODE AND DESCRIPTION OF SYSTEM OPERATION

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SOURCE CODE AND DESCRIPTION OF SYSTEM OPERATION

Certain information is used in several PHAS modules. The numeric and strings variables corresponding to them are declared to be COMMON. These variables are identified in Table A.1.

A.1 Error Traps

PHAS has two general types of traps to handle errors. The first type is for "non-fatal" errors, incorrect inputs which, if accepted by program algorithms, lead to incorrect execution and results. These traps consist of "IF...THEN " statements within the modules that test for the presence of incorrect entries to prompts. These entries include numerics or alphanumerics not specified as input (for example, if "yes" or "no" is expected, but "maybe" is the response). If such an entry is detected, a message is displayed and execution is transferred to either a line which provides information about the input or again requests the input.

The traps that handle "fatal errors" (errors which cause premature and unexpected termination of program execution) are accessed via an "ON ERROR GOTO..." command. The traps are activated by the GWBASIC interpreter error code, and when encountered, an explanation of the likely error is provided. You are usually routed back to a program line preceding the line at which the error was encountered.

Except where traps are of special interest, they will not be discussed further. The author has programmed traps for previously-encountered or anticipated user errors. If you encounter other errors, you are encouraged to contact the author (see Preface for address).

A.2 INSTALL

The code for this stand-alone program appears in Figure A-1. After the "INSTALLATION MENU" is displayed (lines 20-110), you supply an integer value from 1 and 4, which is equated to the variable ENTR. A branching "ON ENTR GOTO..." command at line 130 directs program execution. Values of ENTR of 1, 2 or 3 cause the string TWF\$ to be defined respectively as "B", "A", or ". If ENTR = 4, your supplied drive/subdirectory information is assigned to TWF\$ at line 160. TWF\$ is then written to the file ASSIGN.CMP at line 600. At line 630, you are advised of the value of TWF\$, and the program ends.

Table A.1 COMMON Variables in OPEN11 and Their Functions

PANM\$(140)	Contains alphanumeric designations for the data variables used by the system.
PMT\$(20)	Contains widely-used prompts, messages, filenames, and other alphanumeric statements. PMT\$(7) contains either 'soil' or 'water'; PMT\$(20) is the stored chemical name.
PANV(140)	Contains the numeric values for data variables used in PHAS.
IPATH(30)	Index for cited paths. Locations 1-10 reserved for water-related paths, locations 11-30 reserved for soils-related paths. A value of 1 indicates that a path has been selected; a value of 0 indicates that a path has not been selected.
PAIDEX(140)	Element values are integers from 0 to 4 (see Section 4.5.3). The content of this array comprise the DUST.
LIMIT(10)	Contains miscellaneous numeric values used throughout PHAS.

A.3 OPEN11

The source code for OPEN11 is in Figure A-2. Since this is the entry module, common variable arrays in Table A.1 with more than 10 elements are dimensioned. The strings corresponding to PANM\$ elements (these appear in Appendix B) are down-loaded from file PARAM.CMP at lines 40-50. At line 610, PMT\$(5) is read from ASSIGN.CMP, the file created by INSTALL. PMT\$(5) is the device name of the drive or subdirectory where external data files are located. At lines 630-640, the file PROMPT.CMP is down-loaded from that device. This file contains eight strings, which are read into these PMT\$ elements:

```

PMT$(1)= "      Enter 'yes' or 'no'."
PMT$(2)= "      Input error, try again."
PMT$(3)= "      defalvc.lds ( A default .LDS file)
PMT$(4)= "!!!!Wrong type file, try again."
PMT$(6)= "(80 blank spaces)"
PMT$(7)= "off" ( This is changed to "soil" or "water" during PHAS
           execution. )
PMT$(8)= "defalva.lds" ( A default .LDS file )
PMT$(9)= "defalc.dat" ( The default .DAT file )

```

Line 680 dimensions the string array BLURB\$. This array is used to hold description messages (see below). Line 680 is the line to which other modules return control to OPEN11. At lines 690-770, the "MAIN FUNCTION SELECTION MENU" is displayed. Your input defines the variable IFT, the argument for the "ON IFT GOTO..." command at line 790.

The routines executed in response to selections '1','2' and '6' are in OPEN11. At completion of these selections, control is returned to line 690. Selection

```

10 REM install.bas program to load disk assignments for open11.
20 PRINT "***** INSTALLATION MENU *****"
30 PRINT:PRINT " This program assigns a disk drive or subdirectory for"
40 PRINT " external data files of the PHAS system. Once assigned, the drive"
50 PRINT " or subdirectory will be accessed by the system until this program"
60 PRINT " is again run. Enter an option from 1 to 4....":PRINT
70 PRINT " Input '1' for B: drive (good for a dual-floppy disk system)."

```

Figure A-1. Source Code for INSTALL

```

4 COMMON PAIDEX(),IPATH(),PMT$(),PANM$(),PANV(),LIMIT()
10 REM OPEN11 3/3/89 Version
20 OPTION BASE 1
25 ON ERROR GOTO 3100
30 DIM PAIDEX(140),IPATH(30),PANM$(140),PANV(140),PMT$(20)
40 OPEN "param.cmp" FOR INPUT AS #1
50 FOR J%=1 TO 140:INPUT #1,PANM$(J%):NEXT J%:CLOSE #1
610 OPEN "assign.cmp" FOR INPUT AS #1:INPUT #1,PMT$(5):CLOSE #1
630 OPEN PMT$(5)+"prompt.cmp" FOR INPUT AS #2
635 FOR J%=1 TO 4:INPUT #2,PMT$(J%):NEXT J%
640 FOR J%=6 TO 9:INPUT #2,PMT$(J%):NEXT J%:CLOSE #2
650 CLS: LOCATE 5,5: PRINT " ** POLLUTANT HAZARD ASSESSMENT SYSTEM (PHAS) ***"
660 LOCATE 8,15:PRINT "Version 1.1, March 1989"
680 DIM BLURB$(20) 'ENTRY POINT FOR CHAINS blurbs(20) alpha field for info
690 LOCATE 11,5:PRINT "***** MAIN FUNCTION SELECTION MENU *****":PRINT
695 PRINT TAB(5) "ENTER FUNCTION PERFORMED BY ENTRY"
700 PRINT TAB(5) "1 To get a brief description of the system."
710 PRINT TAB(5) "2 To get a more in-depth description of specific modules."
720 PRINT TAB(5) "3 To do your scenario definition and pathway selections."
730 PRINT TAB(5) "4 To do your non-chemical data selection and editing."
750 PRINT TAB(5) "5 To do your chemical data selection and editing."
760 PRINT TAB(5) "6 To review on-line data and pathway information."
765 PRINT TAB(5) "7 To do PPLV Calculation and constraint analysis."
767 PRINT TAB(5) "9 To do selected Chemical Estimation Methods 'off-line'."
770 PRINT TAB(5) "10 To exit the system."
780 INPUT " ENTER YOUR FUNCTION NUMBER: ",IFT
783 IF IFT<1 OR IFT>10 THEN PRINT PMT$(2):GOTO 780
790 ON IFT GOTO 870,1100,800,810,820,2500,855,860,865,2000

```

Figure A-2. Source Code for OPEN11 (page 1 of 3 pages).

```

800 CHAIN "PATWAY11"
810 CHAIN "INPUTS11"
820 CHAIN "CHMFIL11"
855 CHAIN "COMPUT11"
860 PRINT IFT " is currently an undesignated function, try another." :GOTO 780
865 LIMIT(5)=0:PRINT "Please wait for CHMPRP11; loading takes about
    20 seconds":CHAIN "CHMPRP11"
870 CLS: LOCATE 2,1:PRINT " ***** OVERVIEW OF PHAS PROGRAM MODULES ***** "
875 DUMFILES="overview.cmp":GOSUB 2995
1060 GOSUB 3050
1080 CLS:GOTO 690
1100 CLS:LOCATE 10,15:PRINT "*** SELECT FUNCTION NUMBER FOR DESIRED MODULE ***";
    PRINT
1110 PRINT "   Select 1 for PATWAY11 (Scenario builder)"
1120 PRINT "   Select 2 for INPUTS11 (Non-chemical data processor)"
1130 PRINT "   Select 3 for CHMFIL11 (Chemical data processor)"
1132 PRINT "   Select 4 for COMPUT11 (PPLV and Constraint Analysis)"
1134 PRINT "   Select 5 for Diagnostic Printouts Routines"
1136 PRINT "   Select 6 for CHMPRP11 (Chemical Data Information and Estimates)"
1137 PRINT "   Select 7 to exit without module description"
1140 INPUT " ENTER YOUR FUNCTION NUMBER: ",IFT
1145 IF IFT<1 OR IFT>7 OR IFT<>INT(IFT) THEN PRINT PMT$(2):GOTO 1140
1150 ON IFT GOTO 1160,1300,1390,1420,1450,1600,1080
1160 CLS:LOCATE 2,1:PRINT "**** DESCRIPTION OF SCENARIO BUILDER MODULE ****"
1170 DUMFILES="pathway.cmp":GOSUB 2995:GOTO 1060
1300 CLS:LOCATE 2,1:PRINT "**** DESCRIPTION OF NON-CHEMICAL DATA PROCESSOR ****"
1305 DUMFILES="inputs.cmp":GOSUB 2995:GOTO 1060
1390 CLS:LOCATE 2,1:PRINT "**** DESCRIPTION OF CHEMICAL DATA PROCESSOR ****"
1395 DUMFILES="chemfile.cmp":GOSUB 2995:GOTO 1060
1420 CLS:LOCATE 2,1:PRINT "**** DESCRIPTION OF PPLV AND CONSTRAINT ANALYSIS MODULE****"
1425 DUMFILES="compute.cmp":GOSUB 2995:GOTO 1060
1450 CLS:LOCATE 2,1:PRINT "**** DESCRIPTION OF DIAGNOSTIC PRINTOUT MODULE ****"
1455 DUMFILES="diagnost.cmp":GOSUB 2995:GOTO 1060
1600 CLS:LOCATE 2,1:PRINT "DESCRIPTION OF CHEMICAL PROPERTY ESTIMATIONS MODULE"
1605 DUMFILES="chemprop.cmp":GOSUB 2995:GOTO 1060
2000 PRINT PMT$(1): INPUT " Are you leaving the PHAS? ",OP$
2010 IF OP$<>"yes" AND OP$<>"no" THEN PRINT PMT$(2):GOTO 2000
2020 IF OP$="no" THEN CLS:GOTO 690
2030 CLS:PRINT TAB(20) "**** GOODBYE FROM PHAS - HAVE A NICE DAY ****":SYSTEM
2500 PRINT TAB(5) "***** DISPLAY-PRINT UTILITY MENU *****"
2510 PRINT TAB(5) "Input number for desired printout"
2520 PRINT TAB(5) "Select '1' for pathway status"
2525 PRINT TAB(5) "Select '2' for data use status table (DUST)"
2530 PRINT TAB(5) "Select '3' for values of non-chemical data from .LDS file"
2540 PRINT TAB(5) "Select '4' for values of chemical data from .DAT file"
2560 PRINT TAB(5) "Select '5' for printout of variables from .LDS and .DAT files"
2562 PRINT TAB(5) "      with narrative identities supplied."
2565 PRINT TAB(5) "Select '6' to quit this utility and return to main menu."
2570 INPUT NUMB:IF NUMB<>INT(NUMB) OR NUMB>6 OR NUMB<1 THEN
    PRINT PMT$(2):GOTO 2500
2575 ON NUMB GOTO 2580,2650,2720,2780,2890,1080
2580 PRINT TAB(8)"Water"TAB(18)"Soil #1"TAB(28)"Soil #2"
2585 PRINT TAB(8)"Paths"TAB(18)"Paths"TAB(28)"Paths"
2590 FOR J%=1 TO 10:PRINT J% TAB(8) IPATH(J%) TAB(18) IPATH(J%+10)
    TAB(28) IPATH(J%+20):NEXT J%
2610 PRINT:PRINT " 1st column corresponds to water pathways 1 thru 10.":
    PRINT " 2d column corresponds to soils pathways 1 thru 10."
2611 PRINT " 3d column corresponds to soils pathways 11 thru 20."
2612 PRINT " Current info is from loaded or stored file ..."PMT$(11)
2613 PRINT " If no file, your on-line data is not stored off-line."
2620 GOSUB 3050:GOTO 2500

```

Figure A-2. Source Code for OPEN11 (page 2 of 3 pages)

```

2650 PRINT "#ten #ten+1 #ten+2 #ten+3 #ten+4 #ten+5 #ten+6 #ten+7 #ten+8
#ten+9 #ten+10"
2660 PRINT "(row)": FOR J%=0 TO 13
2670 PRINT J% TAB(6) PAIDEX(10*J%+1) TAB(13) PAIDEX(10*J%+2)
TAB(20) PAIDEX(10*J%+3) TAB(27) PAIDEX(10*J%+4) TAB(34) PAIDEX(10*J%+5)
TAB(41) PAIDEX(10*J%+6) TAB(47) PAIDEX(10*J%+7) TAB(55) PAIDEX(10*J%+8)
TAB(62) PAIDEX(10*J%+9) TAB(69) PAIDEX(10*J%+10)
2680 NEXT J%
2685 PRINT "For data index, read down for tens, add across for units."
2690 PRINT "Thus, item at row 4, #ten+4 (44) is index for Upm
(see manual Table 1)":GOTO 2620
2720 LIMIT(1)=0:LIMIT(2)=17:GOSUB 3000
2730 PRINT " For location, read down side for multiple of 5, then across."
2740 PRINT " Last down-loaded file was ...PMT$(12) ". Data stored in ..."
PMT$(13):PRINT " If blank, data are only accessed on-line.":GOTO 2620
2780 LIMIT(1)=18:LIMIT(2)=27:GOSUB 3000
2810 PRINT " Data is for substance "PMT$(20)
2815 PRINT " For location, read down side for multiple of 5, then across."
2820 PRINT " Last down-loaded file was ...PMT$(14) ". Data stored in ..."
PMT$(15):PRINT " If blank, data are only accessed on-line.":GOTO 2620
2890 IF PANV(1)<>0 AND PANV(126)<>0 THEN 2940
2900 PRINT " WARNING: You may not have valid data":PRINT PMT$(1):
INPUT " Do you wish to continue? ",OP$
2920 IF OP$="no" THEN 2500
2930 IF OP$<>"yes" AND OP$<>"no" THEN PRINT PMT$(2):GOTO 2900
2940 FOR J%=1 TO 140:IF PANV(J%)<=0 THEN 2970 ELSE LPRINT PANM$(J%);PANV(J%)
2970 NEXT J%
2975 LPRINT " Substance is "PMT$(20):GOTO 2500
2995 OPEN DUMFILES FOR INPUT AS #1:FOR J%=1 TO 20:INPUT #1,BLURB$(J%):
NEXT J%:CLOSE #1
2998 FOR J%=1 TO 20:PRINT BLURB$(J%):NEXT J%:RETURN
3000 PRINT "line " TAB(10)" one " TAB(24)" two " TAB(38)" three"
TAB(52)" four" TAB(66)" five"
3010 FOR J%=LIMIT(1) TO LIMIT(2)
3020 PRINT J%*5 "+" ;:PRINT TAB(9) PANV(5*J%+1) TAB(23) PANV(5*J%+2)
TAB(37) PANV(5*J%+3) TAB(51) PANV(5*J%+4) TAB(65) PANV(5*J%+5)
3030 NEXT J%
3040 RETURN
3050 INPUT " Hit enter (return) to continue....",ANI$:RETURN
3100 IF ERR=53 AND ERL=610 THEN PRINT "INSTALL has not been executed. Refer to
User's Guide":PRINT "SORRY, YOU CANNOT PROCEED FURTHER.":SYSTEM
3105 IF ERR=71 AND ERL=630 THEN PRINT "PHAS expects stored data in drive "
PMT$(5):PRINT "Drive is apparently empty. Please correct, then press
return to continue":INPUT ANY$:RESUME 630
3110 IF ERR=53 OR ERR=57 AND ERL=630 THEN PRINT "PHAS expects external data
in drive "PMT$(5):PRINT "Wrong data or wrong disk is in place. Please
correct, then":PRINT " press return to continue.":INPUT ANY$:RESUME 630
3115 IF ERR=76 AND ERL=630 THEN PRINT "Your designation of drive for the
Disk B files " PMT$(5):PRINT "Is apparently incorrect. Try INSTALL
again.":SYSTEM
3120 END

```

Figure A-2. Source Code for OPEN11 (page 3 of 3 pages)

'1' causes the file OVERVIEW.CMP (shown in Figure 2, main text) to be down-loaded and displayed. In the Selection '2' routine, the command "ON IFT GOTO..." at line 1150 is used to reference specific descriptions; here, the argument IFT is supplied at line 1140. The descriptions are down-loaded from ".CMP" files. The string DUMFILE\$ is assigned the specific description filename. The subroutine at lines 2995-2998 down-loads the file contents into the string array BLURB\$, and the 20 elements of BLURB\$ are displayed.

Selection '6' accesses a routine which was initially written as a separate module, and is at lines 2500-2975. Its selection menu is at lines 2500-2565. Your response at line 2570 is the argument NUMB for the "ON NUMB GOTO..." command at line 2575. The options associated with NUMB are:

1. Display the contents of the array IPATH on the monitor and the the last .PTH file either down-loaded or stored.
2. Display the contents of the array PAIDEX on the monitor. This display is across the screen, ten elements to a line (lines 2650-2680).
3. Display non-chemical specific data (PANV(1) through PANV(90)) on the monitor as well as the last .LDS files down-loaded or stored. Line 2720 initializes LIMIT(1) and LIMIT(2), and the subroutine at line 3000 is called. This subroutine (through line 3040) displays the PANV array across the screen, five elements to a line.
4. Display chemical specific data (PANV(91) through PANV(140)) and PMT\$(20), the chemical name on the monitor as well as the last .DAT files down-loaded or stored. These data are displayed similarly to .LDS file data.
5. Print out the PANM\$ string and corresponding values in the PANV array for positive-valued elements and PMT\$(20). The line printer is needed for this selection. Line 2890 tests for non-zero values at elements PANV(1) and PANV(126), two "global variables". If zero values are encountered, this means that neither a .LDS or a .DAT file has been down-loaded during the current session or that both files were not prepared correctly. An advisory warning is displayed at line 2900. The printing occurs at line 2940-2970. Line 2940 line has an initial test to skip zero or negative-valued PANV elements, and only prints the paired PANM\$ and PANV for other elements.
6. Leave the routine and return to the OPEN11 main selection menu.

The remaining selections ('3', '4', '5', '7', and '9') access specific modules via the CHAIN command, which is similar to a FORTRAN "CALL". Prior to "CHAINing" to CHMPRP11 (selection '9'), LIMIT(5) is reset to zero at line 865. CHMPRP11 uses LIMIT(5) to differentiate between prior access from OPEN11 and from CHMFIL11. Since CHMPRP11 is the longest module in PHAS, this CHAIN operation may exceed 10 seconds, particularly for slower (< 8 Mhz) systems.

Four error traps are in OPEN11. The first (line 3100) detects the inability to access PMT\$(5). The others detect the absence of PROMPT.CMP, either as a result of an empty floppy disk drive, a floppy disk drive with the wrong disk, or the wrong subdirectory assignment.

A.4 PATWAY11

The source code for this module is in Figure A-3. In addition to the common variables listed in Table A-1, the following arrays appear in PATWAY11:

PHS(30,140) This matrix holds the index status of variables for each pathway.

PMP\$(30) This string array holds the narrative descriptions of pathways.

SCORE(16) An array used to test for potential duplication of passages in the "PATHWAY SELECTIONS AND DATA NEED SUMMARY" report.

PMP\$ strings are read in for the 8 water-based and 14 soil-based pathways from PATPMP.CMP at line 50. Then, the main mode menu is displayed which asks for your input to IFT at line 140. The option to review stored files is provided at lines 160-180.

After the file review option is exercised (or declined), execution branches at line 200, based on IFT. When IFT = 1, you are prompted for a filename (PMT\$(11), line 210). At lines 240-270, the named file is opened, and the contents are down-loaded respectively to IPATH (30 entries), PAIDEX (140 entries), and PMT\$(7). Next, line 300-320 displays pathways included in the file, those pathways for which IPATH is non-zero (line 300). After this display, execution moves to line 860. Here, information is supplied so that PHAS can recognize that a .PTH file has been down-loaded. The flag for this is LIMIT(3) = 1; the "OR" operation sets the right-hand digit of LIMIT(4) to one. The module exits to OPEN11 at line 910.

If IFT = 2, the module executes the file processing/storage mode. PMT\$(7) is the alphanumeric "soil" or "water" at line 353. Based on the entry, LIMIT(1) and LIMIT(2) are valued. For water, LIMIT(1) = 1 and LIMIT(2) = 10; for soil, 11 and 30, respectively. LIMIT(1) and LIMIT(2) restrict presentation of pathways so soil pathways are not displayed if water pathways are specified and vice versa. Version 1.1 of PHAS has capacity for 10 water pathways and 20 soil pathways.

All elements of the arrays IPATH and PAIDEX are set to zero at line 390. This is necessary to preclude errors at line 490 (see below) which would occur if a .PTH file had been previously down-loaded in the current session. At line 410, a loop from LIMIT(1) to LIMIT(2) is entered. The CRT displays PMP\$(J%) for each non-zero string, and you are prompted to enter yes or no at line 440. Your response values a string OP\$. When OP\$ is "yes", execution is routed to a pathway-specific sub-routine by the "ON J% GOSUB ..." command at line 470. When OP\$ is "no", the next J% is accessed at line 500. Each sub-routine contains the non-zero PHS elements for the J%th pathway. Combinations of elements common to several pathways appear in the subroutines at lines 2500-2920 (for example, PANV(56), PANV(57), and PANV(58) always occur together; see line 2600). At line 480, the return from any sub-routine call of line 470, IPATH(J%) is set equal to 1.

```

2 COMMON PAIDEX(),IPATH(),PMT$( ),PANM$( ),PANV(),LIMIT( )
9 REM PATWAY11 REVISED 8/8/89
20 OPTION BASE 1
35 ON ERROR GOTO 3000
40 DIM PHS(30,140),PMP$(30),SCORE(16)
50 OPEN "patmp.cmp" FOR INPUT AS #1:FOR J%=1 TO 30:INPUT #1,PMP$(J%):NEXT J%:
  CLOSE #1
120 CLS:PRINT "**** WELCOME TO SCENARIO FORMULATION MODULE (PATWAY11) ****"
125 PRINT "***** MODE OF OPERATION SELECTION MENU *****"
130 PRINT "  Input '1' to use a stored .PTH file in the 'load and go' mode"
140 INPUT "  ONLY. Otherwise input '2'. ", IFT
145 IF IFT <> 1 AND IFT <> 2 THEN PRINT PMT$(2):GOTO 130
160 PRINT PMT$(1):INPUT "  Do you want a listing of pathindex files? ",OP$
170 IF OP$<>"no" AND OP$<>"yes" THEN PRINT PMT$(2):GOTO 160
180 IF OP$="no" THEN 200 ELSE CLS:FILES PMT$(5)+".pth":GOSUB 2950
200 IF IFT=2 THEN 350
210 INPUT "  Enter your pathway input file (include .PTH extension) ",PMT$(11)
230 IF RIGHT$(PMT$(11),4)<>".pth" THEN PRINT PMT$(4):GOTO 210
240 OPEN PMT$(5)+PMT$(11) FOR INPUT AS #2
250 FOR J%=1 TO 30: INPUT #2,IPATH(J%): NEXT J%
260 FOR J%=1 TO 140: INPUT #2,PAIDEX(J%): NEXT J%:INPUT #2, PMT$(7):CLOSE #2
280 PRINT "  Pathway file information loaded from "PMT$(5)+PMT$(11)
290 PRINT "  *****PATHWAYS IN " PMT$(5)+PMT$(11)
300 FOR J%=1 TO 30: IF IPATH(J%)=0 THEN 320 ELSE PRINT PMP$(J%):PRINT
320 NEXT J%:GOTO 860
350 PRINT "***** SCENARIO CONSTRUCTION ROUTINE *****"
353 INPUT "  Enter medium for PPLV analysis (soil or water): ",PMT$(7)
355 IF PMT$(7)<>"water" AND PMT$(7)<>"soil" THEN PRINT PMT$(2):GOTO 353
360 IF PMT$(7)="water" THEN LIMIT(1)=1:LIMIT(2)=10:GOTO 390
370 IF PMT$(7)="soil" THEN LIMIT(1)=11:LIMIT(2)=30
390 FOR J%=1 TO 140:PAIDEX(J%)=0:NEXT J%:FOR J%=1 TO 30:IPATH(J%)=0:NEXT J%
405 PAIDEX(1)=1:PAIDEX(2)=1:PAIDEX(126)=1:PAIDEX(127)=1:IPOT=0
410 FOR J%=LIMIT(1) TO LIMIT(2):IF LEN(PMP$(J%))<5 THEN 500
440 LOCATE 16,1 :PRINT PMP$(J%):PRINT PMT$(1):
  INPUT "  Do you want this pathway ? ",OP$
450 IF OP$="no" THEN 495
460 IF OP$ <> "yes" THEN PRINT PMT$(2):SCORE(16)=1:GOTO 495
470 ON J% GOSUB 930,940,950,960,970,980,990,1010,1020,1030,
  1040,1050,1060,1070,1080,1090,1100,1110,1120,1125,1126,1130,1140,1144
480 IPATH(J%)=1:IPOT=IPOT OR IPATH(J%)
490 FOR K%=1 TO 140:PAIDEX(K%)=PAIDEX(K%) OR PHS(J%,K%):NEXT K%
495 LOCATE 16,1:GOSUB 2960:IF SCORE(16)=1 THEN SCORE(16)=0:GOTO 440
500 NEXT J%
504 IF IPOT<>0 THEN 515
505 PRINT "  NO PATHWAYS WERE SELECTED IN THIS RUN. IS THIS WHAT YOU WANT?"
506 INPUT "  Please enter yes or no. ",ANY$
508 IF ANY$<>"yes" AND ANY$<>"no" THEN PRINT PMT$(2):GOTO 505
510 IF ANY$="yes" THEN PRINT "  Program will exit directly to OPEN11":
  GOSUB 2950:GOTO 910
512 PRINT "  Program will go back to pathway display and selection sequence":
  GOSUB 2950
514 LOCATE 16,1:GOSUB 2960:GOTO 410
515 LOCATE 16,10 :PRINT "  NOW PRINTING OUT DATA REQUIREMENTS REPORT"
517 LPRINT:LPRINT "***** PATHWAY SELECTIONS AND DATA NEEDS SUMMARY *****"
520 LPRINT "  FOR ALL PATHWAYS, YOU WILL NEED":LPRINT PANM$(1) " or "PANM$(2)
540 LPRINT TAB(5) "and either":LPRINT PANM$(126)
550 LPRINT " or "PANM$(127)
560 LPRINT:LPRINT " ***** SPECIAL ABBREVIATIONS *****"
562 LPRINT "  dwb = dry weight basis":LPRINT "  nodim = dimensionless"
564 LPRINT "  p.c. = partition coefficient":LPRINT
570 FOR J%=LIMIT(1) TO LIMIT(2):IF IPATH(J%)=0 THEN 640

```

Figure A-3. Source Code for PATWAY11 (page 1 of 4 pages).

```

590 LPRINT PMP$(J%):LPRINT:LPRINT "PRIME VARIABLES INVOLVED IN CALCULATION ARE"
600 FOR K%=3 TO 130: IF PHS(J%,K%)/2 <> INT(PHS(J%,K%)/2) THEN LPRINT PANM$(K%)
620 NEXT K%
630 LPRINT TAB(30) " *****": LPRINT
640 NEXT J%
645 LPRINT:LPRINT "****COMPUTATION OPTIONS FOR CHEMICAL MAIN PATH VARIABLES****"
650 FOR J%=111 TO 125: IF PAIDEX(J%)=0 OR PAIDEX(J%)=2 THEN 670
665 ON (J%-110) GOSUB 1150,1190,1190,1320,1340,1380,1400,1430,1440,1460,1170
670 NEXT J%
672 LPRINT TAB(20) "***** CONSTRAINT ANALYSIS ADVISORY *****"
673 LPRINT TAB(5) "Type 1: PPLV may adversely effect non-human species or
overlook":LPRINT TAB(5) "non-toxic adverse human responses":LPRINT
676 FOR J%=131 TO 140: IF PAIDEX(J%)<>4 THEN 680
679 ON (J%-130) GOSUB 2000,2100,2200,2300,2300,2400,2400,2400
680 NEXT J%
684 IF PMT$(7)="water" THEN LPRINT:LPRINT " Type 2 constraint occurs if PPLV exce
LPRINT PANM$(95):LPRINT:GOTO 695
686 LPRINT:LPRINT " Type 2 constraint occurs if conc. in water phase when soil
conc. = PPLV":LPRINT " Exceeds "PANM$(95):LPRINT
695 PRINT "***** STORAGE DISPOSITION MENU *****"
697 PRINT " Storage to external file routine. You can store the information"
700 PRINT " developed in this session a file on 'Disk 2'. If not,"
705 PRINT " the information is in on-line storage until overwritten."
710 INPUT " Enter '1' for no storage, '2' for file storage. ", IFT
720 IF IFT<>2 AND IFT<>1 THEN PRINT PMT$(2):GOTO 710
730 IF IFT=1 THEN 860 ELSE INPUT " ENTER AN ALLOWABLE NAME UP TO 8
ALPHANUMS ",PMT$(11)
740 IF PMT$(11)="default.pth" THEN PRINT " Please don't use default.pth as a
filename. Try again":GOTO 730
795 IF LEN(PMT$(11))>8 THEN PRINT PMT$(2):GOTO 730
800 FILL$=PMT$(5)+PMT$(11)+".pth":OPEN FILL$ FOR OUTPUT AS #1
820 FOR J%=1 TO 30: WRITE #1,IPATH(J%): NEXT J%
830 FOR J%=1 TO 140: WRITE #1,PAIDEX(J%):NEXT J%:WRITE #1,PMT$(7):CLOSE #1
850 PRINT TAB(5) "You have stored scenario on file "FILL$:PMT$(11)=FILL$
860 GOSUB 2950:LIMIT(3)=1:LIMIT(4)=LIMIT(4) OR LIMIT(3)
910 CLS:CHAIN "open11",680
930 PHS(1,3)=1:PHS(1,131)=4:PHS(1,23)=1:RETURN
940 PHS(2,111)=1:PHS(2,4)=1:PHS(2,24)=1:GOSUB 2750
945 PHS(2,91)=2:PHS(2,101)=2:PHS(2,132)=4:RETURN
950 PHS(3,5)=1:PHS(3,25)=1:PHS(3,112)=1:PHS(3,113)=2:PHS(3,118)=2:PHS(3,91)=2
954 GOSUB 2500:GOSUB 2750:PHS(3,95)=0:RETURN
960 PHS(4,6)=1:PHS(4,26)=1:PHS(4,114)=1:GOSUB 2525:GOSUB 2910
965 GOSUB 2900:PHS(4,106)=2:PHS(4,115)=2:GOSUB 2750:RETURN
970 PHS(5,6)=1:PHS(5,26)=1:GOSUB 2525:GOSUB 2760:GOSUB 2910
973 GOSUB 2900:PHS(5,106)=2:GOSUB 2750:PHS(5,118)=2:GOSUB 2500:RETURN
980 PHS(6,7)=1:PHS(6,27)=1:GOSUB 2550:PHS(6,114)=2:PHS(6,115)=1
982 PHS(6,106)=2:GOSUB 2900:GOSUB 2750:GOSUB 2920:RETURN
990 PHS(7,7)=1:GOSUB 2550:GOSUB 2770:PHS(7,106)=2:GOSUB 2750:GOSUB 2900
994 PHS(7,27)=1:PHS(7,118)=2:GOSUB 2500:GOSUB 2920:RETURN
1010 PHS(8,12)=1:PHS(8,13)=1:PHS(8,33)=1:PHS(8,121)=1:PHS(8,131)=4:RETURN
1020 RETURN 'resv for path9
1030 RETURN 'resv for path10
1040 PHS(11,3)=1:PHS(11,23)=1:PHS(11,59)=1:PHS(11,119)=1
1045 GOSUB 2780:GOSUB 2750:PHS(11,101)=2:PHS(11,131)=4:RETURN
1050 PHS(12,4)=1:PHS(12,24)=1:PHS(12,111)=1:PHS(12,60)=1:PHS(12,119)=1
1053 GOSUB 2750:GOSUB 2780:PHS(12,101)=2:PHS(12,132)=4:RETURN
1060 PHS(13,5)=1:PHS(13,25)=1:PHS(13,112)=1:PHS(13,118)=1:GOSUB 2800
1065 GOSUB 2750:PHS(13,113)=2:GOSUB 2500:RETURN
1070 PHS(14,6)=1:PHS(14,26)=1:PHS(14,118)=1:GOSUB 2800:GOSUB 2760
1072 GOSUB 2900:GOSUB 2750:PHS(14,106)=2:GOSUB 2910:GOSUB 2500:RETURN

```

Figure A-3. Source Code for PATWAY11 (page 2 of 4 pages)

```

1080 PHS(15,6)=1:PHS(15,26)=1:PHS(15,118)=1:GOSUB 2800:GOSUB 2760:GOSUB 2500
1082 GOSUB 2900:PHS(15,106)=2:GOSUB 2750:GOSUB 2910
1086 PHS(15,44)=1:PHS(15,45)=1:RETURN
1090 PHS(16,6)=1:PHS(16,26)=1:PHS(16,45)=1:PHS(16,118)=1
1092 GOSUB 2525:GOSUB 2780:GOSUB 2800:PHS(16,119)=1:GOSUB 2910:PHS(16,106)=2
1094 GOSUB 2900:GOSUB 2750:GOSUB 2760:GOSUB 2500:RETURN
1100 PHS(17,7)=1:PHS(17,27)=1:PHS(17,118)=1:GOSUB 2800:GOSUB 2770:GOSUB 2920
1102 GOSUB 2900:GOSUB 2750:PHS(17,106)=2:GOSUB 2500:RETURN
1110 PHS(18,7)=1:PHS(18,118)=1:GOSUB 2800:PHS(18,47)=1:PHS(18,48)=1:GOSUB 2770
1112 GOSUB 2900:GOSUB 2750:GOSUB 2920:PHS(18,106)=2:GOSUB 2500
1116 PHS(18,27)=1:PHS(18,91)=2:RETURN
1120 PHS(19,7)=1:PHS(19,27)=1:PHS(19,118)=1:GOSUB 2800:GOSUB 2770
1121 GOSUB 2550:PHS(19,48)=1:PHS(19,119)=1:GOSUB 2920
1122 PHS(19,106)=2:GOSUB 2750:GOSUB 2780:GOSUB 2500:GOSUB 2900:RETURN
1125 PHS(20,8)=1:PHS(20,28)=1:RETURN
1126 PHS(21,9)=1:PHS(21,29)=1:RETURN
1130 PHS(22,10)=1:PHS(22,66)=1:PHS(22,67)=1:PHS(22,68)=1:PHS(22,76)=1
1131 PHS(22,80)=1:PHS(22,81)=1:PHS(22,116)=1:PHS(22,117)=1:PHS(22,120)=1
1132 PHS(22,96)=2:PHS(22,92)=2:PHS(22,93)=2:PHS(22,30)=1:PHS(22,77)=1
1133 PHS(22,65)=2:PHS(22,101)=2:GOSUB 2750:RETURN
1140 PHS(23,11)=1:PHS(23,56)=1:GOSUB 2800:PHS(23,78)=1:PHS(23,79)=1
1141 PHS(23,82)=1:PHS(23,83)=1:PHS(23,84)=1:PHS(23,116)=1:PHS(23,117)=1
1142 GOSUB 2750:PHS(23,96)=2:PHS(23,96)=2:PHS(23,31)=1:PHS(23,118)=1
1143 PHS(23,92)=2:PHS(23,93)=2:RETURN
1144 PHS(24,12)=1:PHS(24,13)=1:PHS(24,121)=1:PHS(24,131)=4:GOSUB 2750
1145 PHS(24,59)=1:PHS(24,61)=2:PHS(24,62)=1:PHS(24,63)=1:PHS(24,119)=1
1146 PHS(24,101)=2:PHS(24,33)=1:RETURN
1150 LPRINT PANM$(111):LPRINT TAB(5) " can be estimated as a function of"
1160 LPRINT PANM$(94):LPRINT " or " PANM$(95):LPRINT " or " PANM$(101):LPRINT
1170 RETURN
1190 IF SCORE(2)=1 OR SCORE(3)=1 THEN RETURN
1195 LPRINT PANM$(112):LPRINT TAB(5) " can be estimated by three methods in
PHAS. First,":LPRINT " Kvw = "PANM$(113)
1210 LPRINT " Second, Kvw is function of":LPRINT PANM$(94)
1230 LPRINT " Third, Kvw can be estimated from":LPRINT PANM$(102)
1250 LPRINT " or "PANM$(103)
1260 LPRINT " If soil-water partition coefficient info is available about soil"
1270 LPRINT " used to characterize Ksw or Ksp [ Kd(soil) ],"
1280 LPRINT TAB(10) "Kvw = Ksw x Kd(soil) or Ksp x Kd(soil)"
1290 LPRINT " See Kd2 message for estimation methods of Kd(soil)"
1300 LPRINT " NOTE: Kwp can be estimated by analog, replacing Kvw for Kwp"
1305 LPRINT " above and vice versa.":GOTO 1430
1320 IF SCORE(4)=1 THEN RETURN
1322 LPRINT PANM$(114):LPRINT " can be estimated by two methods.
First, Kpm = Kpat x fm"
1324 LPRINT " where":LPRINT PANM$(106):LPRINT PANM$(41):LPRINT
1326 LPRINT " Next, Kpm = Kpd x (fm/fd), where "
1328 LPRINT PANM$(115):LPRINT PANM$(42):LPRINT
1332 LPRINT:LPRINT " Kpat can be estimated as a function of"
1334 LPRINT PANM$(95)
1336 LPRINT " or "PANM$(94):LPRINT:SCORE(4)=1:RETURN
1340 LPRINT " Estimation approaches for "PANM$(115)
1342 LPRINT " See Kpm writeup for estimation approaches to Kpd."
1344 LPRINT " Make the following switches: Kpd for Kpm; fd for fm"
1346 LPRINT " and fm for fd":LPRINT:GOTO 1320
1360 IF SCORE(7)=1 THEN RETURN
1382 LPRINT PANM$(116):LPRINT " may be estimated by the quotient of"
1383 LPRINT PANM$(96) " divided by":LPRINT PANM$(95):LPRINT:
LPRINT " Several estimation methods are available for each of these."
1384 LPRINT " Water solubility can be estimated from":LPRINT PANM$(94)
1385 LPRINT " Vapor pressure can be estimated from":LPRINT PANM$(93):
LPRINT " For liquids. Generally for solids,"

```

Figure A-3. Source Code for PATWAY11 (page 3 of 4 pages).

```

1386 LPRINT PANM$(92):LPRINT " will be needed. Check CHMPRP11 for more details."
1389 LPRINT:SCORE(7)=1:RETURN
1400 IF SCORE(8)=1 THEN RETURN
1402 LPRINT PANM$(117):LPRINT " can be estimated from molecular components and":LI
1409 LPRINT:SCORE(8)=1:RETURN
1430 LPRINT " Kd2 message for estimation methods applicable to all Kd.":LPRINT
1440 IF SCORE(10)=1 THEN 1449
1443 LPRINT PANM$(119):LPRINT TAB(10) " = Koc x foc + (th2/rh2)":LPRINT
1446 LPRINT PANM$(101):LPRINT TAB(5) " can be estimated as a function of"
1448 LPRINT PANM$(95): LPRINT " or " PANM$(94)
1449 LPRINT:SCORE(2)=1:SCORE(3)=1:SCORE(10)=1:RETURN
1460 IF SCORE(11)=1 THEN RETURN
1462 LPRINT " See Kd2 for estimation approaches to":LPRINT PANM$(120)
1464 LPRINT " Substitute subscript '3' for '2'.":LPRINT:SCORE(11)=1:RETURN
2000 LPRINT " PPLV may have organoleptic (taste,smell) constraint if"
2005 LPRINT PANM$(131) " is in .dat file":LPRINT:RETURN
2100 LPRINT " PPLV may have adverse aquatic biota effect constraint if"
2105 LPRINT PANM$(132) " is in .dat file":LPRINT:RETURN
2200 LPRINT " PPLV may have adverse livestock effect constraint if"
2205 LPRINT PANM$(133) " is in .dat file":LPRINT:RETURN
2300 IF SCORE(15)=1 THEN RETURN
2305 LPRINT " PPLV may have phytotoxic effect constraint if"
2310 LPRINT PANM$(134) " or"
2315 LPRINT PANM$(135) " is in .dat file":LPRINT:SCORE(15)=1:RETURN
2400 RETURN 'reserved for unused values above index 136
2500 FOR K%=101 TO 105:PHS(J%,K%)=2:NEXT K%
2510 FOR K%=134 TO 136:PHS(J%,K%)=4:NEXT K%:RETURN
2525 FOR K%=43 TO 44:PHS(J%,K%)=1:NEXT K%:RETURN
2550 FOR K%=46 TO 47:PHS(J%,K%)=1:NEXT K%:RETURN
2750 PHS(J%,94)=2:PHS(J%,95)=2:PHS(J%,91)=2:RETURN
2760 PHS(J%,112)=2:PHS(J%,113)=1:PHS(J%,114)=1:PHS(J%,115)=2:RETURN
2770 PHS(J%,112)=2:PHS(J%,113)=1:PHS(J%,114)=2:PHS(J%,115)=1:RETURN
2780 PHS(J%,61)=2:PHS(J%,62)=1:PHS(J%,63)=1:RETURN
2800 PHS(J%,56)=2:PHS(J%,57)=1:PHS(J%,58)=1:RETURN
2900 PHS(J%,41)=2:PHS(J%,42)=2:RETURN
2910 PHS(J%,49)=4:PHS(J%,133)=4:RETURN
2920 PHS(J%,50)=4:PHS(J%,133)=4:RETURN
2950 INPUT " Hit enter (return) to continue....",ITY$:RETURN
2960 FOR JJ%=1 TO 6:PRINT PMT$(6):NEXT JJ%:RETURN
3000 IF ERR=53 AND ERL=180 THEN PRINT "Drive accessed "PMT$(5)" does not
contain .pth files":PRINT "Try another disk or move disk to correct
drive":OP$="fff":RESUME 130
3005 IF ERR=71 AND ERL=180 THEN PRINT "Drive accessed "PMT$(5)" is idle.
Please insert correct disk":OP$="fff":RESUME 130
3007 IF ERR=64 OR ERR=75 OR ERR=76 AND ERL=240 THEN PRINT "Entered filename
is defective. Try again. ":RESUME 210
3010 IF ERR=53 AND ERL=240 THEN PRINT "Either file is not on line or disk is
not correct.":PRINT "Will list .pth files on referred disk":OP$="fff":
GOSUB 2950:RESUME 180
3015 IF ERR=71 AND ERL=240 THEN PRINT "Drive accessed "PMT$(5)" does not have
your named file:PRINT "WILL LIST .PTH FILES IF THEY EXIST":OP$="FFF":
GOSUB 2950:RESUME 180
3020 IF ERR=71 AND ERL=800 THEN PRINT "Drive accessed "PMT$(5)" is idle.
Please insert correct disk":RESUME 730
3030 IF ERR=64 OR ERR=75 OR ERR=76 AND ERL=800 THEN PRINT "Entered filename
is defective, try again":RESUME 730
3035 IF ERR=53 AND ERL=800 THEN PRINT "Apparently, path or disk drive cited is
not expected by system":PRINT "Correct path/disk drive is "PMT$(5)"
try again.":RESUME 730

```

Figure A-3. Source Code for PATWAY11 (page 4 of 4 pages)

In line 490, the array PAIDEX is updated to incorporate data roles indicated from each pathway's non-zero PHS entries. PHS(J%,K%) values are either 0, 1, 2 or 4. If the value is 1, PANV(K%) appears in the Pathway J% intake equation (see Section A.7). If the value is 2, PANV(K%) does not appear in the pathway J% intake equation, but can be used to estimate a variable which does. If the value is 4, PANV(K%) is used in a constraint analyses for pathway J%. A restriction employed is that a PHS(J%,K%) of four can be "ORed" only with a PAIDEX(K%) of zero or four. Otherwise, any combination of PHS(J%,K%) OR PAIDEX(K%) values is allowed. The allowed results are:

PAIDEX >>		0	1	2	3	4
		Result of the logical PAIDEX(K%) OR PHS(J%,K%)				
	0	0	1	2	3	4
P	1	1	1	3	3	*
H >>	2	2	3	2	3	*
S	4	4	*	*	*	4

where a "*" indicates an excluded situation. PAIDEX(K%) has the following useful recall properties:

- o If PAIDEX(K%) is odd, at least one PHS(J%,K%) that was "ORed" with it equaled 1.
- o If PAIDEX(K%) is zero, all PHS(J%,K%) that were "ORed" with it equaled 0.
- o If PAIDEX(K%) = 2, none of the PHS(J%,K%) "ORed" with it equaled 1.
- o If PAIDEX(K%) = 4, at least one PHS(J%,K%) "ORed" with it equaled 4.

The PAIDEX array comprises the DUST for the INPUTS11 and CHMFIL11 data processing routines.

After all pathways are so processed, there is a "no path" selection test on line 504. If IPOT = 0, (see lines 405 and 480), no pathways were selected, and PATHWAY11 queries you (line 505-506). If you enter 'yes' at line 506 (see section 4.5.1 concerning review of the pathway descriptions), the module transfers control immediately to OPEN11. If you answer 'no', control is transferred to line 410, so you can again select pathways.

If IPOT = 1 at line 504, execution is transferred to line 515, and the hard-copy printout routine starts. First, global variables (BW, BWc, DT, and DTc) are processed. At line 570, a pathway loop starts, and if IPATH(J%) = 1, the string PMP\$(J%) is printed. At line 600, a nested loop for variables indexed from K% = 3 to 130 is entered. In this loop, if PHS(J%,K%) = 1, the corresponding PANM\$(K%) is printed as the name of a main variable.

At line 650, the variable loop "FOR J%=111 TO 125" is entered. If PAIDEX(J%) is odd, a specific subroutine is entered (line 665) which provides information about how PHAS can estimate the J%th variable. Before a printout sequence which could be duplicated commences, SCORE(J%) is tested. If unity, the sequence is by-passed. At the end of a printout sequence, SCORE(J%) is set equal to one.

At line 676, a loop for constraint data starts. If PAIDEX(J%) = 4 , a sub-routine is entered (line 679) for printouts of constraint information. Last, a message concerning the Type 2 constraint is printed out. PMT\$(7) determines whether the message at line 684 or 686 is printed.

The storage routine starts at line 710 with your input to IFT. If IFT = 1 , control transfers to line 860. Otherwise, you enter a filename PMT\$(11) at line 730. If there are no name errors, the filename string FILL\$ is developed at line 800. Then the arrays IPATH and PAIDEX and the string PMT\$(7) are written to the file (line 820-830). The file name is echoed back at line 850, and after transferring the FILL\$ string to PMT\$(11), execution proceeds to line 860.

A.5 INPUTS11

The source code is in Figure A-4. The array DATDEX(170) holds the DUST within the module. The major operational mode display is at lines 70-90, and your input is the variable IFTA. If you select '1', line 105 tests whether PANV(1) is non-zero. If so, line 105 routes execution to line 70 for another mode input. If not, line 110 directs execution to line 240, which informs of the last down-loaded .LDS file. Line 247 allows you to either continue processing on-line data or to return to line 70 to select another mode operation.

If you selected '2' or '3' as input to IFTA, execution goes to line 120, the option to view .LDS files. At line 170 is the option to use the default file DEFALVA.LDS. A "yes" response equates the string FIL\$ to PMT\$(8) (line 190). Otherwise at line 200, you are prompted to supply FIL\$, the name of the file to be down-loaded. At line 220, the file is down-loaded and its contents become the first 90 elements of the PANV array.

At line 225, the down-loaded filename is included within PMT\$(12). If you are in the "load-and-go" mode, program execution skips to line 650 (see below). Otherwise, execution proceeds to line 240, which was described above. Next, the "DATA USE STATUS TABLE (DUST) LOADING PROCESS MENU" is encountered (line 250-290). Three options are displayed; your response is input to IFT. If IFT = 1 , line 325 tests if PAIDEX(126) = 0 . If so, this indicates some error with the on-line PAIDEX array, and line 260 is accessed for another selection. Otherwise, the first 90 elements of PAIDEX are loaded into DATDEX(1) through DATDEX(90) at line 330. If IFT = 2 , the .PTH file for down-loading to the DATDEX array is specified at 380 after an option to view .PTH files (lines 350-370). At lines 420-430, the 170 numerical values in the selected .PTH file are down-loaded to DATDEX. Since the first 30 entries down-loaded correspond to the the IPATH array, a second loop is entered where the value in DATDEX(31) is transferred to DATDEX(1), and so forth, until DATDEX(120) is so processed (line 440). If IFT = 3 , the line 415 assigns the down-loaded filename as DEFAULT.PTH. Since DATDEX is not a common variable array, the .PTH information in DATDEX is NOT retained on-line after completion of INPUTS11.

The module enters the data review loop at line 480. A given element J% is processed if PANM\$(J%) is not a null (empty) string. The file DEFAULT.PTH

```

5 COMMON PANM$( ), PANV( ), PMT$( ), PAIDEX( ), IPATH( ), LIMIT( )
10 REM INPUTS11 VERSION OF 8/8/89
15 OPTION BASE 1
20 ON ERROR GOTO 680
30 DIM DATDEX(170)
65 CLS:PRINT " WELCOME TO NON-CHEMICAL DATA PROCESSING SUBROUTINE (INPUTS11) "
70 PRINT TAB(10) "***** MAJOR MODE OF OPERATION MENU *****"
75 PRINT " Select '1' to process on-line information (in program memory). "
80 PRINT " Select '2' to use a stored .LDS file in a 'load and go' mode. "
90 INPUT " Select '3' to modify a stored .LDS file. Enter selection: ", IFTA
100 IF IFTA <> 1 AND IFTA <> 2 AND IFTA <> 3 THEN PRINT PMT$(2):GOTO 70
105 IF IFTA=1 AND PANV(1)=0 THEN PRINT "No valid on-line info,
      select another option.":GOTO 70
110 IF IFTA=1 THEN 240
120 PRINT TAB(5) PMT$(1):INPUT " Do you want a listing of files? ", ANI$(1)
130 IF ANI$(1)<>"no" AND ANI$(1)<>"yes" THEN PRINT TAB(5) PMT$(2):GOTO 120
140 IF ANI$(1)="no" THEN 170 ELSE FILES PMT$(5)+".lds":GOSUB 670
170 PRINT TAB(5) PMT$(1):INPUT " Use default file? ", ANI$(2)
180 IF ANI$(2)<>"no" AND ANI$(2)<>"yes" THEN PRINT TAB(5) PMT$(2):GOTO 170
190 IF ANI$(2)="yes" THEN FIL$=PMT$(8):GOTO 220
200 INPUT " Enter file name including .lds extension: ", FIL$
205 IF LEN(FIL$)>12 THEN PRINT "Name too long!!! Try again.":GOTO 200
210 IF RIGHT$(FIL$,4)<>".lds" THEN PRINT "Wrong file type!!! Try again":
      GOTO 170
220 OPEN PMT$(5)+FIL$ FOR INPUT AS #1:FOR J%=1 TO 90:INPUT #1,PANV(J%):
      NEXT J%:CLOSE #1
225 PMT$(12)=PMT$(5)+FIL$:IF IFTA=2 THEN 650
240 PRINT " Last down-loaded file was.....":PRINT " PMT$(12)" . "PMT$(1)
243 PRINT " You may have modified contents since down-loading.
      Continue (yes/no)?":INPUT ANY$
245 IF ANY$<>"yes" AND ANY$<>"no" THEN PRINT PMT$(2):GOTO 240
247 IF ANY$="no" THEN GOTO 70
250 CLS:PRINT "**** DATA USE STATUS TABLE (DUST) LOADING PROCESS MENU *****"
260 PRINT TAB(5) "You will need a DUST to process data. Select 1 of 3 options."
270 PRINT " Select '1' to use the on-line scenario DUST."
275 PRINT " Select '2' to use the DUST from a stored '.PTH' file."
277 PRINT " The program will prompt you for a file name."
280 PRINT " Select '3' to create a new .LDS file for storage or peruse all "
290 INPUT " data in a .LDS file. Enter selection: ", IFT
310 IF IFT <> 1 AND IFT <> 2 AND IFT <> 3 THEN PRINT PMT$(2):GOTO 260
320 ON IFT GOTO 325,350,415
325 IF PAIDEX(126)=0 THEN PRINT "CAUTION! You don't have a valid DUST on line":
      GOTO 260
330 FOR J%=1 TO 90:DATDEX(J%)=PAIDEX(J%):NEXT J%:GOTO 475
350 PRINT TAB(5) PMT$(1):INPUT " Do you wish to see .PTH files? ", OP$
360 IF OP$<>"yes" AND OP$<>"no" THEN PRINT PMT$(2):GOTO 350
370 IF OP$="no" THEN 380 ELSE FILES PMT$(5)+".pth":GOSUB 670
380 INPUT " Input name of file with extension '.pth': ", FIL$
400 IF LEN(FIL$)>12 THEN PRINT "Name too long!!! Try again.":GOTO 380
410 IF RIGHT$(FIL$,4)<>".pth" THEN PRINT PMT$(4):GOTO 380
415 IF IFT=3 THEN FIL$="default.pth"
420 OPEN PMT$(5)+FIL$ FOR INPUT AS #2
430 FOR J%=1 TO 170:INPUT #2,DATDEX(J%):NEXT J%:CLOSE #2
440 FOR J%=1 TO 90:DATDEX(J%)=DATDEX(J%+30):NEXT J%:GOTO 475
475 PRINT "***** DATA REVIEW AND MODIFICATION ROUTINE *****"
480 FOR J%=1 TO 90:IF LEN(PANM$(J%))<1 THEN 560:IF IFT=3 THEN 510
500 IF DATDEX(J%)=0 THEN 560
510 PRINT TAB(5) "*****":PRINT TAB(5) PANM$(J%) " = "PANV(J%)
515 IF DATDEX(J%)=1 OR DATDEX(J%)=3 THEN PMT$(16)= "Main Input Variable"
      ELSE IF DATDEX(J%)=2 THEN PMT$(16)= "Item may be needed to estimate input
      variable" ELSE IF DATDEX(J%)=4 THEN PMT$(16)= "Used in constraint analysis."
516 PRINT " Status in current analysis is: "PMT$(16)

```

Figure A-4. Source Code for INPUTS11 (page 1 of 2 pages)


```

520 PRINT " Enter '1' to accept current value and move on to next variable"
522 INPUT " Enter '2' to change value. Enter choice...",OPT
530 IF OPT=1 THEN 560 ELSE IF OPT<>2 THEN PRINT PMT$(2):GOTO 510
550 INPUT " Enter revised value...",PANV(J%):GOTO 510
560 NEXT J%
565 OPEN "storeit.cmp" FOR INPUT AS #1: FOR J%=1 TO 10:INPUT #1,BLURB$(J%):
PRINT BLURB$(J%):NEXT J%:CLOSE #1
590 INPUT " Enter your selection: ", IFT
600 IF IFT <>0 AND IFT<>1 AND IFT <>2 THEN PRINT TAB(5) PMT$(2):GOTO 565
610 ON IFT+1 GOTO 650,612,615
612 PMT$(13)=PMT$(12):GOTO 640
615 INPUT " Please enter filename (8 alphanums or less, no punct.). ",FLT$
617 IF LEN(FLT$)>8 THEN PRINT "Caution, only 8 characters in filename":GOTO 615
618 IF LEN(FLT$)=0 THEN PRINT "No filename noted, try again":GOTO 615
620 PMT$(13)=PMT$(5)+FLT$+".lds"
640 IF PMT$(13)=PMT$(5)+PMT$(8) OR PMT$(13)=PMT$(5)+"defalvc.lds" THEN
PRINT "Default file writeover not allowed. Try another name":GOTO 615
641 IF ASC(FLT$)<91 THEN PRINT " Please don't use capital letters!":GOTO 615
642 OPEN PMT$(13) FOR OUTPUT AS #3
645 FOR J%=1 TO 90:WRITE #3,PANV(J%):NEXT J%:CLOSE #3
650 PRINT TAB(5) "You down-loaded file "PMT$(12):IF IFTA=2 THEN 656
652 PRINT TAB(5) "You have stored in file ..."PMT$(13) ". If unnamed, this
session's":PRINT TAB(5) "results are only in on-line storage."
656 GOSUB 670:LIMIT(3)=10:LIMIT(4)=LIMIT(4) OR LIMIT(3)
660 CLS:CHAIN "open1",680
670 INPUT " Hit enter (return) key to continue....",ANI$:RETURN
680 IF ERR=53 AND ERL=140 THEN PRINT "System installed to access "PMT$(5):
PRINT "Either redo INSTALL or move data disk":RESUME 120
690 IF ERL=220 AND ERR=53 OR ERR=64 OR ERR=75 OR ERR=76 THEN PRINT "Either file
is not on disk or disk is in wrong drive.":PRINT "System installed to
access "PMT$(5):PRINT "File search will be attempted":ANI$(1)="yes":
RESUME 140
692 IF ERR=53 AND ERL=370 THEN PRINT "Either file is not on disk or disk is in
wrong drive.":PRINT "System installed to access "PMT$(5):PRINT "File search
will be attempted":RESUME 350
693 IF ERL=420 AND ERR=53 OR ERR=64 OR ERR=75 OR ERR=76 THEN PRINT " Incorrect
name, please view directory":OP$="yes":RESUME 370
696 IF ERL=642 AND ERR=53 OR ERR=64 OR ERR=75 OR ERR=76 THEN PRINT " Incorrect
format to name "FLT$" try again.":RESUME 615

```

Figure A-4. Source Code for INPUTS11 (page 2 of 2 pages)

forces all DATDEX elements to be reviewed (line 480). If IFT <> 3 , line 500 is executed, which skips over any Jth element when DATDEX(J%) = 0 . Otherwise, the Jth elements of PANM\$ and PANV are displayed (line 510), along with a statement of use (see Section 4.5.2). For each displayed datum, the option is presented to accept the given value or change the value (line 520-550).

After the data review loop is completed, the "STORAGE DISPOSITION MENU" is displayed. The file STOREIT.CMP is read in to show options (lines 565); your option is placed in IFT (line 590). For no off-line storage, IFT = 0 , and control passes to line 650. If IFT = 1 , line 612 sets PMT\$(13) to PMT\$(12), the device and name for the down-loaded file (this algorithm allows you to "overwrite" the down-loaded .LDS file). Otherwise, at line 615, you input FLT\$, the filename for storage, which at line 620 is used to construct PMT\$(13). Line 640 checks to see if FLT\$ is either "defalva.lds" or "defalvc.lds"; line 641 checks if the first letter in FLT\$ is uppercase. If any of these errors occur, you are informed of this, and sent back to line 615 to provide a different name. These algorithms should prevent overwriting the two default files for most situations.

With a correct filename, the first 90 elements of PANV are written to the file PMT\$(13) (line 645). The down-loaded filename, PMT\$(12), is echoed back (line 650). If you are not in the "load and go" mode, line 652 identifies the stored file (if any). At line 656, LIMIT(4) is "ORed" with LIMIT(3), which has the value 10. This places '1' in the tens position of LIMIT(4). Then, program control passes back to OPEN11.

A.6 CHMFIL11

The code for CHMFIL11 is in Figure A-5. The initial steps of CHMFIL11 are similar to those shown in INPUTS11 with the following noteworthy differences:

- o The default filename is assigned to PMT\$(9); see line 1015
- o DATDEX is declared common for purposes of interactions with CHMPRP11. It contains the DUST for PANV elements processed in CHMFIL11, and here is a 50-element array.
- o CHMFIL11 processes the elements PANV(91) to PANV(140). There is an offset of 90 between DATDEX and PANV in this module's algorithms. When an on-line DUST is used, line 1305 duplicates PAIDEX(91) through PAIDEX(140) in DATDEX(1) through DATDEX(50). If a DUST is down-loaded (lines 1360-1365), the array DUMDEX is used to store the 170 numerical data from the down-loaded .PTH file, and at line 1370, the last 50 data are sequentially assigned to DATDEX. If all PANV are to be viewed, the file DEFAULT.PTH is designated to be down-loaded (line 1350).
- o Prior to exit from CHMFIL11 to OPEN11, LIMIT(4) is "ORed" with LIMIT(3), which equals 100. This places a "1" in the hundreds column of LIMIT(4).
- o The COMMON string variable array STATDEX\$(50) is used to decide which subroutines in CHMPRP11 contain only informational messages and which also contain estimation routines. STATDEX\$ elements are either "yes" or "no", and these strings determine the message shown at line 2056.

The data modification routine in CHMPRP11 is more complex than that in INPUTS11, and involves a "non FOR - NEXT" loop. The routine starts at line 1900, where the counter CTL initially equals 1. Then the contents of the file STATDEX.CMP are down-loaded to the array STATDEX\$. Line 2000 causes display of the routine heading. At lines 2030 and 2040, two conditions directing to line 2200 are provided: if PANM\$(CTL+90) is not defined, and if DATDEX(CTL) is zero. However, if IFT = 3 (assigned at line 1130), the second condition test is bypassed. At line 2200, CTL is increased by one. Line 2200 also checks if CTL = 51; if so, the loop is completed. If neither bypass is executed, the variable name, PANM\$(CTL+90), and value, PANV(CTL+90), is displayed (line 2050) along with its possible role in the scenario (line 2051-2052).

You have three data processing options, which is the variable LUT (lines 2054-2055). Line 2065 checks if LUT is one (accept PANV(CTL+90)); if so, line 2200 is accessed. If LUT = 2, line 2090 requests a manual input of PANV(CTL+90). If LUT = 3, LIMIT(5) is set equal to one, LIMIT(6) to CTL, and CHMPRP11 is

```

5 COMMON PANM$( ),PAIDEX( ),PANV( ),PMT$( ),IPATH( ),LIMIT( ),DATDEX( ),STATDEX( )
10 REM CHMFIL11 REVISED 9/5/89
15 OPTION BASE 1
20 ON ERROR GOTO 5550
25 DIM DUMDEX(170),DATDEX(50),STATDEX$(50)
30 CLS:PRINT "*** WELCOME TO THE CHEMICAL DATA PROCESSING MODULE (CHMFIL11) ****"
35 PRINT:PRINT "***** MAJOR MODE OF OPERATION MENU *****"
40 PRINT " Select '1' to process on-line information (in program memory). "
50 PRINT " Select '2' to used stored .DAT file in a 'load and go' mode."
55 INPUT " Select '3' to modify a stored .DAT file. Enter selection: ",IFTA
60 IF IFTA <>1 AND IFTA <>2 AND IFTA<>3 THEN PRINT PMT$(2):GOTO 35
65 IF IFTA=1 AND PANV(126)=0 THEN PRINT "No valid on-line info!
    Select another option":GOTO 35
70 IF IFTA=1 THEN 1110
100 PRINT PMT$(1):INPUT " Do you want listing of chemical files? ", OP$
200 IF OP$ <> "no" AND OP$ <> "yes" THEN PRINT PMT$(2):GOTO 100
250 CHECKIT$=PMT$(5)+".dat":IF OP$="no" THEN 1005 ELSE FILES CHECKIT$
1005 PRINT PMT$(1):INPUT " Use default chemical file? ",OP$
1010 IF OP$ <> "yes" AND OP$ <> "no" THEN PRINT PMT$(2):GOTO 1005
1015 IF OP$="yes" THEN FIL$=PMT$(9):GOTO 1050
1025 INPUT " Enter chemical data filename including '.dat' extension: ",FIL$
1035 IF LEN(FIL$)>12 THEN PRINT "Too many characters! Try again":GOTO 1010
1040 IF RIGHT$(FIL$,4)<>".dat" THEN PRINT PMT$(4):GOTO 1025
1050 OPEN PMT$(5)+FIL$ FOR INPUT AS #3
1060 FOR J#=1 TO 50:INPUT #3,PANV(J#+90):NEXT J#:INPUT #3,PMT$(20):CLOSE #3
1070 PMT$(14)=PMT$(5)+FIL$:IF IFTA=2 THEN 3900
1080 PRINT " Last down-loaded file was.....":PRINT " PMT$(14)" . "
1090 PRINT " You may have modified contents since down-loading.
    Continue (yes/no)?":INPUT ANY$
1095 IF ANY$<>"yes" AND ANY$<>"no" THEN PRINT PMT$(2):GOTO 1080
1100 IF ANY$="no" THEN GOTO 35
1110 CLS:PRINT "***** DATA USE STATUS TABLE (DUST) LOADING PROCESS MENU *****"
1112 PRINT " You will need a DUST to process data. Select 1 of 3 options."
1115 PRINT " Select '1' to use the on-line scenario DUST."
1117 PRINT " Select '2' to use the DUST from a stored .PTH file"
1120 PRINT " The program will prompt you for a file name."
1121 PRINT " Select '3' to create a new .DAT file for storage or peruse"
1130 INPUT " all data in a .DAT file. Enter selection: ",IFT
1135 IF IFT <>1 AND IFT <>2 AND IFT <>3 THEN PRINT PMT$(2):GOTO 1112
1140 ON IFT GOTO 1300,1310,1350
1300 IF PAIDEX(126)=0 THEN PRINT "CAUTION! You do not have a valid index on
    line.":GOTO 1112
1305 FOR J#=1 TO 50:DATDEX(J#)=PAIDEX(J#+90):NEXT J#:GOTO 1900
1310 PRINT TAB(5) PMT$(1) :INPUT"Do you want to see .PTH files? ",OP$
1315 IF OP$ <> "yes" AND OP$ <> "no" THEN PRINT PMT$(2):GOTO 1310
1320 IF OP$="no" THEN 1330 ELSE FILES PMT$(5)+".pth":GOSUB 4500
1330 INPUT "Input name of file with extension '.pth' ":FILES$
1335 IF LEN(FILES$)>12 THEN PRINT "name too long, try again":GOTO 1330
1340 IF RIGHT$(FILES$,4) <> ".pth" THEN PRINT PMT$(4):GOTO 1330
1350 IF IFT=3 THEN FILES$="default.pth"
1360 OPEN PMT$(5)+FILES$ FOR INPUT AS #1
1365 FOR J#=1 TO 170: INPUT #1,DUMDEX(J#):NEXT J#:CLOSE #1
1370 FOR J#=1 TO 50: DATDEX(J#)=DUMDEX(J#+120):NEXT J#:GOTO 1900
1900 CTL=1:OPEN "statdex.cmp" FOR INPUT AS #1
1910 FOR J#=1 TO 50:INPUT #1,STATDEX$(J#):NEXT J#:CLOSE #1
2000 PRINT "***** DATA REVIEW AND MODIFICATION ROUTINES *****"
2030 IF LEN(PANM$(CTL+90))<1 THEN 2200:IF IFT=3 THEN 2050
2040 IF DATDEX(CTL)=0 THEN 2200
2050 PRINT TAB(5) "*****":PRINT TAB(2) PANM$(CTL+90) " = "PANV(CTL+90)
2051 IF DATDEX(CTL)=1 OR DATDEX(CTL)=3 THEN PMT$(16)="Main input variable"
    ELSE IF DATDEX(CTL)=2 THEN PMT$(16)="Item may be needed to estimate input
    variable" ELSE IF DATDEX(CTL)=4 THEN PMT$(16)="Used in constraint analysis"

```

Figure A-5. Source Code for CHMFIL11 (page 1 of 2 pages)

```

2052 PRINT " Status in scenario is:"PMT$(16)
2053 PRINT: PRINT " Select '1' to accept value."
2054 PRINT " Select '2' to insert new value."
2055 PRINT " Select '3' to enter estimation routine for value
2056 IF STATDEX$(CTL)="yes" THEN PRINT " Estimation routine available." ELSE
PRINT " Information only available."
2057 PRINT: INPUT " Enter your selection: ",LUT
2062 IF LUT<>1 AND LUT<>2 AND LUT<>3 THEN PRINT PMT$(2):GOTO 2053
2065 IF LUT=1 THEN 2200
2090 IF LUT=2 THEN INPUT " Input revised value."; PANV(CTL+90):GOTO 2050
2100 IF LUT=3 THEN LIMIT(5)=1:LIMIT(6)=CTL:CHAIN "chmprp11"
2200 CTL=CTL+1:IF CTL<51 GOTO 2030
2210 PRINT TAB(5) "Is chemical name "PMT$(20)" ok? ":INPUT OP$
2215 IF OP$="yes" THEN 3800
2220 IF OP$ <> "no" THEN PRINT PMT$(2):GOTO 2210
2230 LINE INPUT "Input revised name: ",PMT$(20):GOTO 2210
3800 OPEN "storeit.cmp" FOR INPUT AS #1:FOR J%=1 TO 10:INPUT #1,BLURB$(J%):
PRINT BLURB$(J%):NEXT J%:CLOSE #1
3830 INPUT " Enter your selection: ",IFT
3840 IF IFT<>0 AND IFT<>1 AND IFT<>2 THEN PRINT PMT$(2):GOTO 3800
3850 ON IFT+1 GOTO 3920,3855,3860
3855 PMT$(15)=PMT$(14):GOTO 3880
3860 INPUT " Please enter filename (8 alphanums or less,no punct.) ";FIL$
3862 IF LEN(FIL$)>8 THEN PRINT "Only 8 characters in filename. Try again":
GOTO 3860
3864 IF LEN(FIL$)=0 THEN PRINT "No filename noted, try again":GOTO 3860
3870 PMT$(15)=PMT$(5)+FIL$+".dat"
3880 OPEN PMT$(15) FOR OUTPUT AS #2
3890 FOR J%=1 TO 50:WRITE #2,PANV(J%+90):NEXT J%:WRITE #2,PMT$(20):CLOSE #2
3900 PRINT " You down-loaded file "PMT$(14):IF IFTA=2 THEN GOTO 3920
3902 PRINT " You stored in file ..." PMT$(15)
3905 PRINT " If unnamed, session's results are on-line until over-written."
3920 LIMIT(3)=100:LIMIT(4)=LIMIT(4) OR LIMIT(3):GOSUB 4500
4000 CLS:CHAIN "open11",680
4500 INPUT " Press enter (return) key to continue....",IKY$:RETURN
5000 CTL=LIMIT(6):GOTO 2050
5550 IF ERR=53 AND ERL=300 THEN PRINT "System installed to access "PMT$(5):
PRINT "Either redo INSTALL.EXE or move data disk":RESUME 100
5555 IF ERL=1050 AND ERR=53 OR ERR=64 OR ERR=75 OR ERR=76 THEN PRINT "Either
file is not on disk or disk is in wrong drive.":PRINT "System installed
to access"PMT$(5):PRINT "File search to be attempted":OP$="ff":RESUME 300
5560 IF ERL=1360 AND ERR=53 OR ERR=64 OR ERR=75 OR ERR=76 THEN PRINT "Either
file is not on disk or disk is in wrong drive.":PRINT "System installed
to access"PMT$(5):PRINT "File search to be attempted":OP$="ff":RESUME 1320
5570 IF ERL=3880 AND ERR=53 OR ERR=75 OR ERR=76 THEN PRINT "Incorrect format to
name, try again":RESUME 3860

```

Figure A-5. Source Code for CHMFIL11 (page 2 of 2 pages).

accessed (line 2100). If CHMPRP11 produces an estimate of PANV(CTL+90), when CHMFIL11 is re-entered (line 5000), the estimate will be PANV(CTL+90). If an estimate is not computed in CHMPRP11, PANV(CTL+90) is unchanged. Line 5000 "resets" CTL; since LIMIT(6) is common, its value is retained when CHMPRP11 chains back to CHMFIL11. Control is unconditionally transferred to line 2050 where the variable name and value are again displayed for further processing.

After this routine is complete, the storage disposition algorithm is executed, which parallels that of INPUTS11. PMT\$(14) contains the name of the last down-loaded file from CHMFIL11 in the current session, and PMT\$(15) contains the name of the file selected to store processed data (if so desired). As discussed above, line 3920 carries out the "OR" operation with LIMIT(4), and at line 4000, control returns to OPEN11.

A.7 COMPUT11

The code for COMPUT11 is in Figure A-6. Several arrays are dimensioned for exclusive use in COMPUT11. These are:

- o INTAKE, with 41 elements. Elements 1-40 hold computed intakes due to the presence of 1 mg/L pollutant in water or 1 mg/kg pollutant in soil. Elements 1-30 correspond to pathways. Element 41 sums the 40 intakes.
- o PROMP\$, with 40 elements. Short pathway descriptions are placed in this array (see lines 55-85).
- o C2DEX, with 40 elements. Each element corresponds to an element in the INTAKE array. C2DEX indexes whether a pathway or portion of a pathway is subject to a Type 2 constraint status at the PPLV concentration (see Section A.7.3).
- o CTAKE and NTAKE, each with 41 elements. These arrays are used in the Type 2 constraint analysis to keep track of constrained and non-constrained intakes needed to adjust the PPLV.
- o BLURB\$, with 20 elements, used to hold down-loaded file information.

Execution starts at line 315, where LIMIT(4) is tested to see if there is a non-zero number in the digits column. If not, control passes to line 350. Otherwise, the contents of a .PTH file are on-line, and this information is used if you respond "yes" at line 320. Then control passes to line 510. If no information is on-line or on-line information is not wanted, the option to review .PTH files occurs at line 350. At line 400, you supply a filename (PMT\$(11) for down-loading, and at lines 440 and 450, the contents of file PMT\$(11) are down-loaded into the IPATH and PAIDEX arrays, and the string PMT\$(7). Since these variables are common, they are in on-line storage.

The above algorithm is repeated for .LDS and .DAT files. At lines 515 and 705 respectively, the tests to check for the presence of on-line information about non-chemical and chemical data are executed. If on-line information is not present, control passes to lines 550 or 900, respectively. If on-line information is there, it can be selected by responding "yes" at lines 520 or 750, respectively. Otherwise, the .LDS file selected at line 600 is down-loaded at line 620 and its contents assigned to PANV(1) through PANV(90); the .DAT file selected at line 1100 is down-loaded at line 1150-1225 and its contents assigned to PANV(91) through PANV(140) and to PMT\$(20).

A.7.1 The PPLV Analysis Algorithm

At line 1300, IFT is entered; it determines the limiting intake ADITAKE to be the basis for the PPLV calculation; see line 1350. Line 1360 bypasses two soil PPLV computation options if PMT\$(7) = "water". The option to compute three Kd values (as the product of Koc and the appropriate foc) is presented at line 1400. You set IFT = 1 to do this; line 1410 is executed. The option to compute Kpm = Kpat x fm and Kpd = Kpat x fd directly is then presented at line 1575. You set IFT = 1 to do this; line 1625 is executed.

```

5 COMMON PANM$( ), PAIDEX( ), PANV( ), PMT$( ), IPATH( ), LIMIT( )
10 REM COMPUT11.BAS version of 12/8/89
20 OPTION BASE 1:ON ERROR GOTO 9900
40 DIM INTAKE(41), PROMP$(40), C2DEX(40), CTAKE(41), NTAKE(41), BLURB$(20)
50 CLS:PRINT:PRINT "*** WELCOME TO THE PHAS PPLV COMPUTATION MODULE COMPUTE1 ***"
55 PROMP$(1) = "Drink Water":PROMP$(2) = "Eat Fish":PROMP$(3) = "Eat Vegetables"
60 PROMP$(4) = "Eat Beef [W]":PROMP$(5) = "Eat Beef [W+P]"
62 PROMP$(8) = "Dermal Abs":PROMP$(24) = "Dermal Abs":PROMP$(7) = "Drink Milk [W+P]"
65 PROMP$(11) = "Drink Water":PROMP$(12) = "Eat Fish":PROMP$(13) = "Eat Vegetables"
70 PROMP$(14) = "Eat Beef [P]":PROMP$(15) = "Eat Beef [P+S]":PROMP$(16) =
  "Eat Beef [P+S+W]":PROMP$(6) = "Drink Milk [W]"
75 PROMP$(17) = "Drink Milk [P]":PROMP$(18) = "Drink Milk [P+S]":
  PROMP$(19) = "Drink Milk [P+S+W]"
80 PROMP$(20) = "Norm. Soil/Dust":PROMP$(21) = "Heavy Soil/Dust"
85 PROMP$(22) = "Diffusing vapor/inside":PROMP$(23) = "Diffusing vapor/outside"
300 PRINT "***** SCENARIO SELECTION *****"
315 IF INT(LIMIT(4)/10) = LIMIT(4)/10 THEN 350
320 PRINT PMT$(1):INPUT "      Do you want on-line DUST info? ", OP$
330 IF OP$ <> "yes" AND OP$ <> "no" THEN PRINT PMT$(2):GOTO 320
340 IF OP$ = "yes" THEN 510
350 PRINT PMT$(1):INPUT "      Do you want to see .PTH files? ", OP$
360 IF OP$ <> "no" AND OP$ <> "yes" THEN PRINT PMT$(2):GOTO 350
370 IF OP$ = "no" THEN 400 ELSE FILES PMT$(5)+".pth":GOSUB 9600
400 INPUT "      Enter file name including '.pth' extension: ", PMT$(11)
410 IF RIGHT$(PMT$(11),4) <> ".pth" THEN PRINT PMT$(4):GOTO 400
440 OPEN PMT$(5)+PMT$(11) FOR INPUT AS #1:FOR J%=1 TO 30:INPUT #1, IPATH(J%):
  NEXT J%
450 FOR J%=1 TO 140:INPUT #1, PAIDEX(J%):NEXT J%:INPUT #1, PMT$(7):CLOSE #1
510 PRINT "***** NON-CHEMICAL SPECIFIC DATA SELECTION *****"
515 IF INT(LIMIT(4)/10) <> 1 AND INT(LIMIT(4)/10) <> 11 THEN 550
520 PRINT PMT$(1):INPUT "      Do you want on-line non-chem input data? ", OP$
530 IF OP$ <> "yes" AND OP$ <> "no" THEN PRINT PMT$(2):GOTO 520
540 IF OP$ = "yes" THEN 700
550 PRINT PMT$(1):INPUT "      Do you want to see .LDS files? ", OP$
560 IF OP$ <> "yes" AND OP$ <> "no" THEN PRINT PMT$(2):GOTO 550
570 IF OP$ = "no" THEN 600 ELSE FILES PMT$(5)+".lds":GOSUB 9600
600 INPUT "      Enter file name including '.lds' extension: ", PMT$(12)
610 IF RIGHT$(PMT$(12),4) <> ".lds" THEN PRINT PMT$(4):GOTO 600
620 OPEN PMT$(5)+PMT$(12) FOR INPUT AS #1:FOR J%=1 TO 90:INPUT #1, PANV(J%):
  NEXT J%:CLOSE #1
700 PRINT "***** CHEMICAL-SPECIFIC DATA SELECTION *****"
705 IF LIMIT(4) - 99 < 0 THEN 900
750 PRINT PMT$(1):INPUT "      Do you want on-line chemical input data? ", OP$
800 IF OP$ <> "yes" AND OP$ <> "no" THEN PRINT PMT$(2):GOTO 750
850 IF OP$ = "yes" THEN 1250
900 PRINT PMT$(1):INPUT "      Do you want to see .DAT files? ", OP$
950 IF OP$ <> "yes" AND OP$ <> "no" THEN PRINT PMT$(2):GOTO 900
1000 IF OP$ = "no" THEN 1100 ELSE FILES PMT$(5)+".dat":GOSUB 9600
1100 INPUT "      Enter file name including '.dat' extension: ", PMT$(14)
1120 IF RIGHT$(PMT$(14),4) <> ".dat" THEN PRINT PMT$(4):GOTO 1100
1150 OPEN PMT$(5)+PMT$(14) FOR INPUT AS #1
1225 FOR J%=91 TO 140:INPUT #1, PANV(J%):NEXT J%:INPUT #1, PMT$(20):CLOSE #1:CLS
1250 PRINT "***** HUMAN TARGET SELECTION *****"
1275 PRINT "      Input '1' if an adult target is to be selected"
1300 INPUT "      Input '2' is a child target is to be selected. Input: ", IFT
1325 IF IFT <> 1 AND IFT <> 2 THEN PRINT PMT$(2):GOTO 1250
1350 IF IFT = 1 THEN ADITAKE = PANV(1)*PANV(126) ELSE ADITAKE = PANV(2)*PANV(127)
1360 IF PMT$(7) = "water" THEN GOTO 1700
1375 PRINT "***** OPTION TO COMPUTE KD = KOC x FOC *****"
1380 PRINT "      This option is recommended for pre-packed .DAT files where the"

```

Figure A-6. Source Code for COMPUT11 (page 1 of 6 pages)

Figure A-6. Source Code for COMPUT11 (page 2 of 6 pages)

```

2970 INTAKE(15)=INTAKE(31)+INTAKE(32):RETURN
3000 INTAKE(31)=PANV(6)*PANV(26)*PANV(114)*((PANV(113)/KDONE)
3010 INTAKE(32)=PANV(6)*PANV(26)*PANV(114)*((PANV(45)/PANV(44))
3020 INTAKE(33)=PANV(6)*PANV(26)*PANV(114)*((PANV(43)/(PANV(44)*KDTWO))
3030 INTAKE(16)=INTAKE(31)+INTAKE(32)+INTAKE(33):RETURN
3050 INTAKE(17)=PANV(7)*PANV(27)*PANV(115)*PANV(113)/KDONE:RETURN
3100 INTAKE(34)=PANV(7)*PANV(27)*PANV(115)*((PANV(113)/KDONE)
3110 INTAKE(35)=PANV(7)*PANV(27)*PANV(115)*((PANV(48)/PANV(47))
3120 INTAKE(18)=INTAKE(34)+INTAKE(35):RETURN
3150 INTAKE(34)=PANV(7)*PANV(27)*PANV(115)*((PANV(113)/KDONE)
3160 INTAKE(35)=PANV(7)*PANV(27)*PANV(115)*((PANV(48)/PANV(47))
3170 INTAKE(36)=PANV(7)*PANV(27)*PANV(115)*((PANV(46)/(PANV(47)*KDTWO))
3180 INTAKE(19)=INTAKE(34)+INTAKE(35)+INTAKE(36):RETURN
3200 INTAKE(20)=PANV(8)*PANV(28):RETURN
3250 INTAKE(21)=PANV(9)*PANV(29):RETURN
3300 DASN=PANV(117)*PANV(68)^(10/3):DAS=DASN/(PANV(68)+PANV(67))^2
3305 COF1=1000*PANV(116)/KDTH
3310 COF2=((PANV(68)+PANV(67)/PANV(116)+PANV(66)*KDTH/PANV(116))*DAS)^.5
3315 TERM1=PANV(81)*COF1*COF2/(3.1416*PANV(81))^.5
3316 TERM0=PANV(80)*COF1*COF2/(3.1416*PANV(80))^.5
3320 FAVN=(TERM1-TERM0)*21/(PANV(81)-PANV(80))
3325 INTAKE(22)=PANV(10)*PANV(30)*PANV(77)*FAVN/PANV(76):RETURN
3350 DASN=PANV(117)*PANV(64)^(10/3):DAS=DASN/(PANV(64)+PANV(58))^2
3355 COF1=1000*PANV(116)/KDONE
3360 COF2=((PANV(64)+PANV(58)/PANV(116)+PANV(57)*KDONE/PANV(116))*DAS)^.5
3365 TERM1=PANV(84)*COF1*COF2/(3.1416*PANV(84))^.5
3370 TERM0=PANV(83)*COF1*COF2/(3.1416*PANV(83))^.5
3375 FAVN=(TERM1-TERM0)*2/(PANV(84)-PANV(83))
3380 INTAKE(23)=FAVN*PANV(82)*PANV(11)*PANV(31)/(86400*PANV(78)*PANV(79)):
RETURN
3400 INTAKE(24)=10*PANV(12)*PANV(13)*PANV(33)*PANV(121)*PANV(59)/KDTWO:RETURN
4000 PRINT "*****CONSTRAINT ANALYSIS *****"
4003 PRINT:PRINT TAB(5) " TYPE 1 CONSTRAINT. For reference, PPLV =" PPLV;UNITS
4010 FOR J%=LIMIT(1) TO LIMIT(2):IF IPATH(J%)=0 THEN 4200
4030 FOR K%=131 TO 140:IF PAIDEX(K%)<>4 OR PANV(K%)<0 THEN 4100
4050 ON J% GOSUB 5100,5200,5300,5400,5500,5600,5700,5800,5900,6000,
6100,6200,6300,6400,6500,6600,6700,6800,6900,7000,7100,7200,7300,7400
4100 NEXT K%
4200 NEXT J%
4202 IF PMTS(7)="water" THEN 4210
4203 PRINT " *****NOTE***** If no test messages were displayed concerning"
4204 PRINT " Type 1 Constraint, no soil pathways other than pathways 10"
4205 PRINT " through 13 were included in the scenario."
4210 PRINT " End Type 1 Constraint Analysis":GOSUB 9600:
IF IFT=1 THEN 2239 ELSE 7500
5100 ON (K%-130) GOSUB 5110,5120,5120,5120,5120,5120,5120,5120,5120:RETURN
5110 PRINT " Test for water pathway # 1 "PROMP$(1)
5111 TEST=PANV(131):GOSUB 9500
5112 IF TEST>PPLV THEN PRINT " PPLV OK FOR ORGANOLEPTIC EFFECTS PROTECTION":
RETURN
5114 PRINT TAB(5) "POTENTIAL CONSTRAINT: offensive drinking water"
5120 RETURN
5200 ON (K%-130) GOSUB 5120,5220,5120,5120,5120,5120,5120,5120:RETURN
5220 PRINT " Test for water pathway # 2 "PROMP$(2)
5221 TEST=PANV(132):GOSUB 9500
5225 IF TEST>PPLV THEN PRINT " PPLV OK FOR AQUATIC BIOTA":RETURN
5230 PRINT TAB(5) "POTENTIAL CONSTRAINT:aquatic biota effects" :RETURN
5300 ON (K%-130) GOSUB 5120,5120,5120,5310,5350,5120,5120,5120:RETURN
5310 PRINT " Test for water pathway # 3 "PROMP$(3)
5311 TEST=PANV(134):GOSUB 9500
5320 IF TEST>PPLV THEN PRINT " PPLV OK FOR PLANTS(based on water data)":
GOSUB 9600:RETURN

```

Figure A-6. Source Code for COMPUT11 (page 3 of 6 pages)

42.

```

5325 PRINT TAB(5) "POTENTIAL CONSTRAINT:plant damage":GOSUB 9600:RETURN
5350 KWS=PANV(136)*PANV(101):TEST=PANV(135)/KWS:GOSUB 9500
5372 IF TEST>PPLV THEN PRINT " PPLV OK FOR PLANTS(based on soil data)":
      GOSUB 9600:RETURN
5375 PRINT TAB(5) "POTENTIAL CONSTRAINT:plant damage.":GOSUB 9600:RETURN
5400 ON (K4-130) GOSUB 5120,5120,5410,5120,5120,5120,5120,5120:RETURN
5410 PRINT " Test for water pathway # 4 "PROMP$(4)
5415 TEST=PANV(49)*PANV(133)/PANV(43):GOSUB 9500
5425 IF TEST>PPLV THEN PRINT " PPLV OK FOR LIVESTOCK":GOSUB 9600:RETURN
5430 PRINT TAB(5) "POTENTIAL CONSTRAINT:livestock adverse effects":
      GOSUB 9600:RETURN
5500 ON (K4-130) GOSUB 5120,5120,5510,5311,5350,5120,5120,5120:RETURN
5510 PRINT " Test for water pathway # 5 "PROMP$(5)
5515 TEST=PANV(49)*PANV(133)/(PANV(43)+PANV(113)*PANV(44)):GOSUB 9500:GOTO 5425
5600 ON (K4-130) GOSUB 5120,5120,5610,5120,5120,5120,5120,5120:RETURN
5610 PRINT " Test for water pathway # 6 "PROMP$(6)
5615 TEST=PANV(50)*PANV(133)/PANV(46):GOSUB 9500:GOTO 5425
5700 ON (K4-130) GOSUB 5120,5120,5710,5311,5350,5120,5120,5120:RETURN
5710 PRINT " Test for water pathway # 7 "PROMP$(7)
5715 TEST=PANV(50)*PANV(133)/(PANV(46)+PANV(113)*PANV(47)):GOSUB 9500:GOTO 5425
5800 ON (K4-130) GOSUB 5810,5120,5120,5120,5120,5120,5120,5120:RETURN
5810 PRINT " Test for water pathway # 8 "PROMP$(8):GOTO 5111
5900 RETURN 'path 9
6000 RETURN 'path10
6100 ON (K4-130) GOSUB 6110,5120,5120,5120,5120,5120,5120,5120:RETURN
6110 PRINT " Test for soil pathway # 1 "PROMP$(11)
6111 TEST= PANV(131)*KDTWO/PANV(59):GOSUB 9500:GOTO 5112
6200 ON (K4-130) GOSUB 5120,6210,5120,5120,5120,5120,5120,5120:RETURN
6210 PRINT " Test for soil pathway # 2 "PROMP$(12)
6215 TEST=PANV(132)*KDTWO/PANV(60):GOSUB 9500:GOTO 5225
6300 ON (K4-130) GOSUB 5120,5120,5120,6310,6350,5120,5120,5120:RETURN
6310 PRINT " Test for soil pathway # 3 "PROMP$(13)
6315 TEST=PANV(134)*KDONE:GOSUB 9500:GOTO 5320
6350 KWS=PANV(136)*PANV(101):TEST=PANV(135)*KDONE/KWS:GOSUB 9500:GOTO 5372
6400 ON (K4-130) GOSUB 5120,5120,6410,6315,6350,5120,5120,5120:RETURN
6410 TEST=PANV(49)*PANV(133)/BCIP:GOSUB 9500:GOTO 5425
6500 ON (K4-130) GOSUB 5120,5120,6510,6315,6350,5120,5120,5120:RETURN
6510 PRINT " Test for soil pathway # 5 "PROMP$(15)
6515 TEST=PANV(49)*PANV(133)/(BCIP+PANV(45)):GOSUB 9500:GOTO 5425
6600 ON (K4-130) GOSUB 5120,5120,6610,6315,6350,5120,5120,5120:RETURN
6610 PRINT " Test for soil pathway # 6 "PROMP$(16)
6615 TEST=PANV(49)*PANV(133)/(BCIP+PANV(45)+(PANV(43)/KDTWO)):
      GOSUB 9500:GOTO 5425
6700 ON (K4-130) GOSUB 5120,5120,6710,6315,6350,5120,5120,5120:RETURN
6710 PRINT " Test for soil pathway # 7 "PROMP$(17)
6711 TEST=PANV(50)*PANV(133)/DCIP:GOSUB 9500:GOTO 5425
6800 ON (K4-130) GOSUB 5120,5120,6810,6315,6350,5120,5120,5120:RETURN
6810 PRINT " Test for soil pathway # 8 "PROMP$(18)
6815 TEST=PANV(50)*PANV(133)/(DCIP+PANV(48)):GOSUB 9500:GOTO 5425
6900 ON (K4-130) GOSUB 5120,5120,6910,6315,6350,5120,5120,5120:RETURN
6910 PRINT " Test for soil pathway # 9 "PROMP$(19)
6917 TEST=PANV(50)*PANV(133)/(DCIP+PANV(48)+(PANV(46)/KDTWO)):
      GOSUB 9500:GOTO 5425
7000 PRINT " No Type 1 constraints for soil pathway # 10 "PROMP$(20):RETURN
7100 PRINT " No Type 1 constraints for soil pathway # 11 "PROMP$(21):RETURN
7200 PRINT " No Type 1 constraints for soil pathway # 12 "PROMP$(22):RETURN
7300 PRINT " No Type 1 constraints for soil pathway # 13 "PROMP$(23):RETURN
7400 ON (K4-130) GOSUB 7410,5120,5120,5120,5120,5120,5120,5120:RETURN
7410 PRINT " Test for soil pathway # 14 "PROMP$(24):GOTO 6111
7500 PRINT "***** TYPE 2 CONSTRAINT ANALYSIS *****"
7505 PRINT:PRINT " For reference, " PANM$(95) " = "PANV(95):
      PRINT " PPLV = " PPLV

```

Figure A-6. Source Code for COMPUT11 (page 4 of 6 pages).

```

7510 IF PMT$(7)="soil" THEN GOTO 7600
7520 IF PPLV<PANV(95) THEN PRINT " PPLV not subject to Type 2 constraint":
      GOSUB 9600:GOTO 2239
7525 PRINT " PPLV exceeds solubility limit. Type 2 constraint exists"
7530 PRINT " Criteria levels in excess of the PPLV may be justified.":GOTO 2239
7600 FOR J%=11 TO 30:C2DEX(J%)=IPATH(J%):NEXT J%
7605 IF IPATH(15)=1 THEN C2DEX(31)=1:C2DEX(32)=1
7610 IF IPATH(16)=1 THEN C2DEX(31)=1:C2DEX(32)=1:C2DEX(33)=1
7615 IF IPATH(18)=1 THEN C2DEX(34)=1:C2DEX(35)=1
7620 IF IPATH(19)=1 THEN C2DEX(34)=1:C2DEX(35)=1:C2DEX(36)=1
7630 REM This space reserved for expansion purposes
7700 ANYNO=0:FOR J%=11 TO 40:IF C2DEX(J%)=0 THEN 7750
7707 C2T$="no"
7710 ON J%-10 GOSUB 9010,9020,9030,9040,9050,9060,9070,9080,9090,9100,
      9110,9120,9130,9140,9150,9150,9150,9150,9150,9150,
      9210,9220,9230,9240,9250,9260,9150,9150,9150,9150
7715 IF C2DEX(J%)=2 THEN C2T$="yes":ANYNO=1
7720 PRINT "Path " PROMP$(J%) " type 2 constraint status = "C2T$
7750 NEXT J%
7751 PRINT "****NOTE**Expect non-defined pathways if pathways 5 or 6 or 8 or 9"
7752 PRINT " were in scenario.":GOSUB 9600
7755 IF ANYNO=1 THEN PRINT " Type 2 constraint flagged, PPLV adjustment
      attempted":GOTO 7800
7795 PRINT " Solubility will not pose a type 2 constraint":GOTO 2239
7800 CNTR=0:FOR J%=11 TO 40:IF C2DEX(J%)<>1 THEN 7810 ELSE CNTR=CNTR+C2DEX(J%)
7810 NEXT J%
7811 IF CNTR<>0 THEN 7815
7812 PRINT " PPLV may not be applicable. System totally constrained.":GOTO 2239
7815 FOR J%=1 TO 41:CTAKE(J%)=0:NTAKE(J%)=0:NEXT J%
7820 FOR J%=LIMIT(1) TO LIMIT(2):IF C2DEX(J%)=0 THEN 7850
7830 IF C2DEX(J%)=1 THEN NTAKE(J%)=PPLV*INTAKE(J%):GOTO 7850
7840 ON J%-10 GOSUB 9310,9320,9330,9340,9350,9360,9370,9380,9390,9400,
      9410,9420,9430,9440
7850 NEXT J%
7860 FOR J%=11 TO 40:CTAKE(41)=CTAKE(41)+CTAKE(J%):
      NTAKE(41)=NTAKE(41)+NTAKE(J%):NEXT J%
7880 RADITAKE=ADITAKE-CTAKE(41):PLV2=PPLV*RADITAKE/NTAKE(41)
7890 PRINT " Adjusted PPLV is "PLV2 " mg/kg."
7900 PRINT " Now checking to see if further adjustment is needed":
      RATPLV=PLV2/PPLV
7910 IF RATPLV<1.001 THEN PRINT " No further adjustment needed.
      Analysis over.":GOTO 2239
7930 PPLV=PLV2:GOTO 7700
9010 IF PPLV*PANV(59)/KDTWO>PANV(95) THEN C2DEX(11)=2:RETURN ELSE RETURN
9020 IF PPLV*PANV(60)/KDTWO>PANV(95) THEN C2DEX(12)=2:RETURN ELSE RETURN
9030 IF PPLV/KDONE>PANV(95) THEN C2DEX(13)=2:RETURN ELSE RETURN
9040 IF PPLV/KDONE>PANV(95) THEN C2DEX(14)=2:RETURN ELSE RETURN
9050 IF PPLV/KDONE>PANV(95) THEN 9055 ELSE RETURN
9055 C2DEX(15)=2:C2DEX(31)=2:RETURN
9060 IF PPLV/KDONE>PANV(95) THEN 9065 ELSE RETURN
9065 C2DEX(16)=2:C2DEX(31)=2:RETURN ELSE RETURN
9070 IF PPLV/KDONE>PANV(95) THEN C2DEX(17)=2:RETURN
9080 IF PPLV/KDONE>PANV(95) THEN 9085 ELSE RETURN
9085 C2DEX(18)=2:C2DEX(34)=2:RETURN
9090 IF PPLV/KDONE>PANV(95) THEN 9095 ELSE RETURN
9095 C2DEX(19)=2:C2DEX(34)=2:RETURN
9100 RETURN
9110 RETURN
9120 IF PPLV/KDTH>PANV(95) THEN C2DEX(22)=2:RETURN ELSE RETURN
9130 IF PPLV/KDONE>PANV(95) THEN C2DEX(23)=2:RETURN ELSE RETURN
9140 IF PPLV*PANV(59)/KDTWO>PANV(95) THEN C2DEX(24)=2:RETURN ELSE RETURN
9150 RETURN 'default return for unused pathways

```

Figure A-6. Source Code for COMPUT11 (page 5 of 6 pages)

```

9210 RETURN 'second part of pathway 15(soil)
9220 RETURN 'second part of pathway 16(soil)
9230 IF PPLV/KDTWO>PANV(95) THEN C2DEX(33)=2
9235 RETURN 'water intake part of 16
9240 RETURN 'second part of pathway 18(soil)
9250 RETURN 'second part of pathway 19(soil)
9260 IF PPLV/KDTWO>PANV(95) THEN C2DEX(36)=2
9265 RETURN 'water intake part of 19
9310 CTAKE(11)=PANV(95)*PANV(3)*PANV(23):RETURN
9320 CTAKE(12)=PANV(95)*PANV(4)*PANV(24)*PANV(111):RETURN
9330 CTAKE(13)=PANV(95)*KDONE*INTAKE(13):RETURN
9340 CTAKE(14)=PANV(95)*KDONE*INTAKE(14):RETURN
9350 NTAKE(32)=PPLV*INTAKE(32)
9351 IF C2DEX(31)=2 THEN CTAKE(31)=PANV(95)*KDONE*INTAKE(31):RETURN
9352 NTAKE(31)=PPLV*INTAKE(31):RETURN
9360 NTAKE(32)=PPLV*INTAKE(32)
9362 IF C2DEX(31)=2 THEN CTAKE(31)=PANV(95)*KDONE*INTAKE(31):GOTO 9366
9364 NTAKE(31)=PPLV*INTAKE(31)
9366 IF C2DEX(33)=2 THEN CTAKE(33)=PANV(95)*KDTWO*INTAKE(33):RETURN
9368 IF C2DEX(33)=1 THEN NTAKE(33)=PPLV*INTAKE(33):RETURN
9370 CTAKE(17)=PANV(95)*KDONE*INTAKE(17):RETURN
9380 NTAKE(35)=PPLV*INTAKE(35)
9381 IF C2DEX(34)=2 THEN CTAKE(34)=PANV(95)*KDONE*INTAKE(34):RETURN
9382 NTAKE(34)=PPLV*INTAKE(34):RETURN
9390 NTAKE(35)=PPLV*INTAKE(35)
9392 IF C2DEX(34)=2 THEN CTAKE(34)=PANV(95)*KDONE*INTAKE(34):GOTO 9396
9394 NTAKE(34)=PPLV*INTAKE(34)
9396 IF C2DEX(36)=2 THEN CTAKE(36)=PANV(95)*KDTWO*INTAKE(36):RETURN
9398 IF C2DEX(36)=1 THEN NTAKE(36)=PPLV*INTAKE(36):RETURN
9400 RETURN 'Not needed since C2DEX(20) always 1 if not 0
9410 RETURN 'Not needed since C2DEX(21) always 1 if not 0
9420 CTAKE(22)=PANV(95)*KDTW*INTAKE(22):RETURN
9430 CTAKE(23)=PANV(95)*KDONE*INTAKE(23):RETURN
9440 CTAKE(24)=PANV(95)*KDTWO*INTAKE(24):RETURN
9500 PRINT "TEST based on "PANM$(K4):PRINT "CRITICAL CONC. = "TEST " " UNIT$:
RETURN
9600 INPUT "Hit enter (return) to continue....",ANY$:RETURN
9900 IF ERL=440 AND ERR=53 OR ERR=64 OR ERR=76 THEN PRINT "File "PMT$(11)"
does not exist on disk. Disk will be":PRINT "checked out. Review and
input correct name.":OP$="ff":RESUME 370
9910 IF ERL=620 AND ERR=53 OR ERR=64 OR ERR=76 THEN PRINT "File "PMT$(12)"
does not exist on disk. Disk will be":PRINT "checked out. Review and
input correct name.":OP$="ff":RESUME 570
9920 IF ERL=1150 AND ERR=53 OR ERR=64 OR ERR=76 THEN PRINT "File "PMT$(14)"
does not exist on disk. Disk will be":PRINT "checked out. Review and
input correct name.":OP$="ff":RESUME 1000
9999 END

```

Figure A-6. Source Code for COMPUT11 (page 6 of 6 pages)

At line 1700, LIMIT(1), LIMIT(2), and the string UNIT\$ are valued based on PMT\$(7). At line 1800, the pathway loop is entered. If IPATH(J%) = 0, line 1900-1950 is skipped; pathway J% is not part of the scenario. If pathway J% is part of the scenario, the "ON J% GOSUB ..." command at line 1900 is executed, and the corresponding INTAKE(J%) is computed. The computation subroutines are between lines 2250 through 3400. Elements INTAKE(31) through INTAKE(40) are reserved for sub-units of soil pathways where animals obtain pollutant through multiple routes. For example, at line 2970, INTAKE(15), the intake of pollutant in meat, is the sum of two other intakes, INTAKE(31) which involves pollutant in plant matter consumed by the beef cow, and INTAKE(32), which involves pollutant in soil ingested by the beef cow. These are computed at lines 3000 and 3010. At line 1950, INTAKE(41) sums all computed intakes.

At lines 2010-2090, the results of the above computations are printed. The PPLV is computed at line 2037 as $ADITAKE/INTAKE(41)$. The SPLV is computed at line 2070, which for path J% is $ADITAKE/INTAKE(J\%)$. The term $INTAKE(J\%)*PPLV$ is the mg/day intake of pollutant at the PPLV concentration; the sum of these terms is ADITAKE.

At the conclusion of the PPLV computation and printout, the file CONTTALK.CMP is down-loaded (line 2100). This file provides information about and the options for Type 1 and Type 2 constraint analysis. You input IFT, the argument for the "ON IFT+1 GOTO..." command at line 2180. Regardless of the IFT selected, lines 2239 is the last line executed in COMPUT11. At this line, LIMIT(4) is set equal to 111. This will inform COMPUT11, when next entered in a current session, that scenario, non-chemical, and chemical data are in on-line storage. Moreover, these data are in an on-line storage status for review or modification in the OPEN11, PATWAY11, INPUTS11, and CHMFIL11 modules, as is applicable.

A.7.2 Type 1 Constraint Analysis

The selection of IFT of one or three sends control to line 4000, where the Type 1 constraint analysis begins. At line 4010, a loop from LIMIT(1) to LIMIT(2) starts; pathways not used in the scenario indicated by IPATH are culled out at line 4020. For each used pathway, a nested loop starts at line 4030 ($K\% = 131$ to 140 , the indices of the constraint data variables). Constraints which are either not relevant or for which data are not available are culled out at line 4030. For constraints which pass these two tests, the "ON J% GOSUB...." command at line 4050 is executed. For each subroutine specified at line 4050, a nested "ON ($K\%-130$) GOSUB..." command line appears, which directs execution to the relevant test for the $K\%$ th index constraint for the $J\%$ th pathway.

The location of these tests is in lines 5110 through 7300. Each test involves determining a water or soil intake corresponding to the constraint. For example, at line 6515, the constraint for cattle intake (mg substance per day) is $PANV(49) \times PANV(133)$, which the animal obtains from pasture and soil. The term: $PANV(49) \times PANV(133) / (BCIP + PANV(45))$ represents the soil concentration which would provide the constrained intake (see line 1777 for BCIP). At the end of each test, the variable TEST is computed. The value is displayed by "GOSUB 9500" routine. Prior to the return to the pathway level, TEST is contrasted to PPLV. If $TEST > PPLV$, a line with format: IF $TEST > PPLV$ THEN PRINT "PPLV OK FOR...." is displayed. Otherwise, the message "POTENTIAL CONSTRAINT:..." is presented. When all relevant, valued constraints for a given $J\%$ th pathway are tested, the next pathway is addressed. An exception to this occurs when any of the soil pathways 20-23 are in the scenario. For each of these pathways, the GOSUB call at line 4050 causes a display of an applicable statement at lines 7000-7300.

A.7.3 Type 2 Constraint Analysis

If $IFT = 1$ (line 2110), the Type 1 constraint analysis is completed when line 4210 is reached. When IFT is two or three, execution is transferred to line 7500. The Type 2 constraint analysis for the water medium is simple; if the

PPLV exceeds a substance's solubility limit, a constraint exists (line 7520). With this test, the module completes execution. If the medium is soil, processing starts at line 7600, where the array C2DEX is reinitialized; C2DEX(J%) = 1 when IPATH(J%) = 1. Moreover, C2DEX elements corresponding to subpaths 31-36 (these deal with the role of soil and water uptake by beef and dairy cows for soil pathways 4, 5, 7, or 8) are valued at lines 7605-7620.

At line 7700, the counter ANYNO is initialized to zero, and a loop "FOR J% = 11 to 40" starts. The status of C2DEX(J%) is checked; when C2DEX(J%) = 0, the loop is incremented. Within this loop, the string C2T\$ is initially "no". If C2DEX(J%) = 1, the "ON J%-10 GOSUB..." command at line 7710 is executed.

The cited subroutines are at lines 9010 to 9260. In each subroutine, the water concentration corresponding to the soil PPLV concentration is computed. If the water level exceeds PANV(95), the solubility limit, C2DEX(J%) is reset to two. The return from each subroutine is to line 7715, which sets C2T\$ to "yes" and ANYNO = 1 whenever C2DEX(J%) = 2. Line 7720 reports the constraint status for the path, and at line 7750, the loop is completed.

If there are no paths subject to a type 2 constraint, control passes to line 7795 and then to line 2239. Otherwise, an adjustment of the PPLV is attempted. Before this attempt, a check is made to see if ALL pathways are constrained; if so, no adjustment can be logically made (see next paragraph). This check is done at lines 7800-7812. A counter CNTR is initialized as zero. A loop on pathways is entered. For each C2DEX(J%) currently equal to one, the ELSE statement at line 7800 increments CNTR by one. At the end of the loop, if CNTR = 0 (only possible if all C2DEX elements are two), line 7812 displays a statement that no adjustment can be made, and control passes to line 2239.

The logic to the PPLV adjustment algorithm is based on the concept that a Type 2-constrained pathway cannot "deliver" the intake expected at the PPLV. Each such pathway "delivers" the intake indicated by water solubility limitations. Thus, if the soil limit were higher than the PPLV, unconstrained pathways can "deliver" more intake, so that the summed intake by all pathways is still ADITAKE. The pathways which can provide more intake at a soil limit > PPLV are those for which C2DEX(J%) = 1.

The adjustment process starts at line 7820, where the pathway loop is entered. In the loop, NTAKE(J%) is evaluated if C2DEX(J%) = 1 (line 7830). However, if C2DEX(J%) = 2, the "ON J% GOSUB..." command at line 7840 is executed. In each subroutine (lines 9310 to 9430), the intake corresponding to the constrained portion of each pathway, CTAKE(J%), is computed. For pathways dealing with cattle ingesting soil or drinking water in addition to eating contaminated plant matter, part of a pathway may be constrained. For example, INTAKE(32) at line 3010 deals with the substance intake in meat attributed to the soil consumed by the beef cow. Subpath 32 cannot be constrained, thus at line 9360, NTAKE(32) is unconditionally computed. At line 9351, CTAKE(31) is computed if C2DEX(31) = 2; otherwise, at line 9352, NTAKE(31) is computed. CTAKE elements are computed for those pathways which are totally or in part constrained. NTAKE elements are computed for non-constrained pathways and those parts of constrained pathways which are not constrained.

At the conclusion of these subroutines, CTAKE(41) and NTAKE(41) are computed, respectively they are the sums of the other elements of the CTAKE and NTAKE arrays. The intake per unit substance concentration after removal of intake "delivered" by constrained pathways or constrained portions of pathways is identified as RADITAKE at line 7880. Then, this line computes PLV2, the adjusted soil level.

However, the PLV2 computed above may not be the final adjustment. The current version of PHAS includes three Kd's; in COMPUT11, they are called KDONE for topsoil, KDTWO for sediment, and KDTH for mixed top and sub-soils. Assume some scenario with pathways, and consider the incidence of Type 2 constraints as a substance concentration in soil is increased. Generally, pathways with KDTH in their calculation equations will be constrained first, then pathways with KDONE, and lastly, those with KDTWO. Conceptually, if PLV2 replaces the PPLV as a soil level, since $PPLV < PLV2$, pathways or portions of pathways that were not constrained at the PPLV may become constrained at a higher concentration level. Thus, an algorithm is included to readjust PLV2 for such a situation.

This process starts at line 7900, where RATPLV is computed. If $RATPLV < 1.001$, no readjustment is needed, and module execution ends (line 7910). Otherwise, at line 7930, PPLV is replaced with PLV2. At this point, execution moves to line 7700 which repeats the valuation of the C2DEX array, this time based on PLV2 rather than PPLV. The algorithm continues to recalculate the CTAKE and NTAKE arrays, the reduced intake RADITAKE, the adjusted soil limit, PLV2, and finally, the ratio RATPLV. The program ends when the test at line 7910 is logically "yes", where control is transferred to line 2239.

A.8 CHMPRP11

A.8.1 The Main Routine

CHMPRP11 is designed to be modular. Its main routine, as discussed here, provides access to 24 component estimation or informational subroutines. The code for the main routine is in Figure A.7. As noted in Section A.6, the COMMON statement includes the arrays DATDEX and STATDEX\$. The components of the DIM statement will be discussed as they occur.

At line 50, the value of LIMIT(5) is checked. If zero, entry to CHMPRP11 is from OPEN11, and control passes to line 200. At line 225, CATLIST.CMP is specified for down-loading and display (Figure 13, main text). This is the selection menu for CHMPRP11. Your response values SELECT (line 550). At line 625, the "ON SELECT GOSUB ..." command directs execution to the estimation or information subroutine corresponding to SELECT. The return to the main routine is at line 650, where the user is queried if he wishes to stay in CHMPRP11. If so (OP\$ is "yes"), line 700 directs execution back to line 200, for the initial menu display. If OP\$ is "no", line 710 chains to OPEN11.

If at line 50, LIMIT(5) = 1, entry to CHMPRP11 is from CHMFIL11. The value of LIMIT(6), the common variable passed from CHMFIL11 to indicate the index of the current PANV element, is checked. If less than 25*, line 60 is executed; otherwise, line 90 is executed. Either line has a "ON LIMIT(6) GOSUB..." command. The return to the main routine is at line 100. If a subroutine is entered and no calculation occurs, the variable SLN will be zero. Its value is tested at line 100; if zero, control passes to line 650. Otherwise, the result carried out of the subroutine is the variable ANSWER. At line 100, the value in ANSWER is transferred to PANV(90+LIMIT(6)), and control passes to line 650. Lines 700-710 contains the algorithm for further processing based on OP\$. When OP\$ is "yes", execution moves to line 50.

A.8.2 Subroutine Structure

At the beginning of each subroutine, an information screen is displayed. To conserve space in the CHMPRP11 source code, the information is in a .CMP file (see Figure 3, main text for a listing of such files). A common subroutine is used to down-load and display these files. BLURB\$ is a 21-element string array. The last element, BLURB\$(21), is assigned the filename to down-load. When required, a GOSUB call is made to either line 15400 (which causes a heading to be displayed) or line 15550. At line 15600, the subroutine down-loads 19 lines from the file into the first 19 elements of BLURB\$, which is printed at line 15650.

Informational subroutines: The molecular weight subroutine is a typical example, and is shown in Figure A-7. Three assignments are made at line 725. PNTR is the index for the property (91 for molecular weight). BLURB\$(21) is the filename for the information screen (in this case, MOLWT.CMP). The variable SK governs whether a halt is executed after a screen is displayed;

* The number of arguments is limited by the 255 character command line limit.

```

2 COMMON PANM$( ),PAIDEX( ),PANV( ),PMT$( ),IPATH( ),LIMIT( ),DATDEX( ),STATDEX( )
10 REM CHMPRP11. 9/5/89 version.
30 OPTION BASE 1
32 ON ERROR GOTO 30000
35 DIM FRAG$(41),VON(41),TON(41),PON(41),MOW(41),NOF(41),KF(40),
    LBAS(22),NOLB(22),LBA$(22),BLURB$(21)
50 IF LIMIT(5)=0 THEN 200 ELSE IF LIMIT(6)>25 THEN 90
60 ON LIMIT(6) GOSUB 725,1350,1450,1400,775,2725,5000,5000,5000,5000,
    5025,5450,5725,5750,5750,4525,5000,5000,5000,5000,5975,6275,6950,6975,7725
70 GOTO 100
90 ON LIMIT(6)-25 GOSUB 8450,9275,10450,10450,10450,11010,5000,5000,5000,
    5000,11050,11100,5000,5000,5000,11150,11200,11300,11600,11700,
    5000,5000,5000,5000,5000
100 IF SLN=0 THEN 650 ELSE PANV(90+LIMIT(6))=ANSWER :GOTO 650
200 CLS:PRINT "*** WELCOME TO THE CHEMICAL PROPERTIES ESTIMATION MODULE *****"
225 BLURB$(21)="catlist.cmp":SK=1:GOSUB 15550
550 INPUT " Input the number of your selection: ",SELECT
575 IF INT(SELECT)<>SELECT THEN PRINT PMT$(2):GOTO 550
600 IF SELECT<1 OR SELECT>31 THEN PRINT "Selection out of number range.
    Try again":GOTO 550
625 ON SELECT GOSUB 725,1350,1450,1400,775,2725,4500,4975,5000,5025,5450,
    5725,5750,1325,5975,6275,6950,4525,6975,7725,8450,9275,10450,11010,
    11050,11100,11150,11200,11300,11600,650
650 PRINT TAB(5) PMT$(1): INPUT "Wish to Do More? ", OP$:
675 IF OP$<>"yes" AND OP$<>"no" THEN PRINT PMT$(2):GOTO 650
700 IF OP$="yes" AND LIMIT(5)=0 THEN GOTO 200 ELSE IF OP$="yes" THEN GOTO 50
710 IF LIMIT(5)=0 THEN CLS:CHAIN "open11",680 ELSE CLS:CHAIN "chmf111",5000
.....
725 PNTR=91:BLURB$(21)="molwt.cmp":SK=1:GOSUB 15400:SLN=0:RETURN
.....
15400 CLS:PRINT "***** INFORMATION ON *****"
15450 PRINT PANM$(PNTR)
15500 FOR J%=1 TO 19:PRINT PMT$(6):NEXT J%
15550 OPEN BLURB$(21) FOR INPUT AS #1
15600 FOR J%=1 TO 19:INPUT #1,BLURB$(J%):NEXT J%:CLOSE #1
15650 LOCATE 4,1:FOR J%=1 TO 19:PRINT BLURB$(J%):NEXT J%
15675 IF SK=1 THEN RETURN ELSE GOSUB 15850:RETURN
15750 IF LIMIT(5)=0 THEN INPUT " Enter Log Kow: ",LKOW:RETURN
    ELSE LKOW=PANV(94):PRINT PANM$(94) " = " PANV(94):RETURN
15775 IF LIMIT(5)=0 THEN INPUT " Enter Mol Weight: ",MWT:
    RETURN ELSE MWT=PANV(91):PRINT PANM$(91) " = " PANV(91):RETURN
15800 PRINT TAB(5) PANM$(PNTR) " = " ANSWER:RETURN
15825 IF LIMIT(5)=0 THEN INPUT " Enter water sol. in mg/L: ",WSOL:RETURN
    ELSE WSOL=PANV(95):PRINT PANM$(95) " = " PANV(95):RETURN
15850 INPUT " Press enter (return) key to continue....",IKY$:RETURN

```

Figure A-7. Source Code for the Main Routine and the Information Display Subroutines of CHMPRP11.

it is when SK = 1 (line 15675). Line 15450 displays PANM\$. At the return from the display subroutine, SLN is set equal to zero. The return to the main routine is to either line 100 (entry from CHMFIL11) or directly to line 650 (entry from OPEN11).

Subroutines with Estimation Methods: These will be discussed below in turn. In general, they are structured as follows:

- o The first line has an assignment of PNTR, BLURB\$(21), and SK. An information screen is displayed as described above.
- o A menu of estimation methods is displayed, from which you select a numerical option. The number is assigned the variable name SLN.

o If you select $SLN = 0$, execution is transferred to the subroutine's final RETURN statement.

o A selection of any other valid SLN transfers execution to the specific estimation method.

o Data input statements that access information from the PANV array have a standardized format (below, VARVALU is a generic term assigned to an element in the PANV array):

```
IF LIMIT(5)=0 THEN INPUT ["prompt for variable"] ,VARVALU
ELSE VARVALU=PANV(index of variable): PRINT.... [:RETURN]
```

Variables used in several estimation routines are accessed by GOSUB calls to lines 15750, 15775, and 15825. In those cases, the "RETURN" is included in the statement. If $LIMIT(5) = 0$ (entry to CHMPRP11 from OPEN11), manual input of data is requested. The ELSE portion provides for transfer of data from the appropriate PANV array element when $LIMIT(5) = 1$.

o At the end of the method's algorithm, ANSWER is computed and displayed by the "GOSUB 15800" command. After this display, the subroutine's RETURN to the main routine occurs.

A.8.3 The Boiling Point Estimation Subroutine

The code for this subroutine is presented in Figure A-8. Line 1450 has assignments of PNTR, BLURB\$(21), and SK, and the GOSUB call to display information. The method is selected in response to the prompt at lines 1500-1575. The selection $SLN = 1$ sends operations to line 1650. The melting point is called MELT . The main calculation occurs at line 1675 (TBOIL in °K):

$$TBOIL = 1.713*(MELT+273.2)$$

ANSWER is the °C counterpart of TBOIL.

If $SLN = 2$ is selected, the numerical parameters for Miller's Method are down-loaded from "MILTBOIL.CMP" at lines 1700-1725. The various variables which appear in the subroutine for this purpose are:

FRAG\$(J%) describes the fragment for the J%th element. There are 41 such elements.

TON(J%), PON(J%), VON(J%), and MOW(J%) are the temperature, pressure, volume, and molecular weight increments of FRAG\$(J%).

NOF(J%) is the number of FRAG\$(J%) in the molecule. Initially, this is valued at zero for all fragments.

An information screen of Miller's Method is down-loaded from "MILLERM.CMP" at line 1750. If you choose to do the computation after reading the message (the option to leave is at lines 1775-1825), the tableau shown in Figure A-9

```

1450 PNTR=93:BLURB$(21)="tboil.cmp":SK=0:GOSUB 15400
1500 PRINT "***** BOILING POINT ESTIMATION MENU *****"
1525 PRINT: PRINT TAB(5) "Select '0' to exit without calculation
1550 PRINT TAB(5) "Select '1' to do 'down and dirty' estimation"
1575 INPUT "      Select '2' to do Miller's method. Enter selection: ",SLN
1600 IF SLN <>0 AND SLN <>1 AND SLN <>2 THEN PRINT PMT$(2):GOTO 1500
1625 ON SLN+1 GOTO 2700,1650,1700
1650 CLS:IF LIMIT(5)=0 THEN INPUT " Enter Melting Point (DegC): ",MELT
      ELSE MELT=PANV(92):PRINT PANM$(92) " = " PANV(92)
1675 TBOIL=1.713*(MELT+273.2): ANSWER=TBOIL-273.2:GOTO 2675
1700 OPEN "MILTBOIL.CMP" FOR INPUT AS #1
1725 FOR J%=1 TO 41: INPUT #1,FRAG$(J%),TON(J%),PON(J%),VON(J%),MOW(J%)
1740 NOF(J%)=0:NEXT J%:CLOSE #1
1750 BLURB$(21)="millerm.cmp":CLS:SK=1:GOSUB 15550
1775 LOCATE 22,5:PRINT PMT$(1):INPUT " Do you wish to continue analysis? ",OP$
1800 IF OP$<>"yes" AND OP$<>"no" THEN PRINT PMT$(2):GOTO 1775
1825 IF OP$="no" THEN 2700
1850 CLS:LOCATE 1,20:PRINT "MILLER BOILING POINT METHOD FRAGMENTS ID TABLE"
1875 FOR J%=0 TO 9:LOCATE J%+2,1:PRINT USING "###";NOF(4*J%+1)
1925 LOCATE J%+2,4:PRINT FRAG$(4*J%+1)
1950 LOCATE J%+2,21:PRINT USING "###";NOF(4*J%+2)
1975 LOCATE J%+2,24:PRINT FRAG$(4*J%+2)
2000 LOCATE J%+2,41:PRINT USING "###";NOF(4*J%+3)
2025 LOCATE J%+2,44:PRINT FRAG$(4*J%+3)
2050 LOCATE J%+2,61:PRINT USING "###";NOF(4*J%+4)
2075 LOCATE J%+2,64:PRINT FRAG$(4*J%+4)
2100 NEXT J%
2125 LOCATE 12,1:PRINT USING "###";NOF(41):LOCATE 12,4:PRINT FRAG$(41)
2150 ZIT%=0:FOR J%=1 TO 41:ZIT%=ZIT%+NOF(J%):NEXT J%
2175 IF ZIT%=0 THEN 2275
2200 LOCATE 20,5:PRINT PMT$(1):INPUT " Do you want to do more? ",ANY$
2225 IF ANY$<>"yes" AND ANY$<>"no" THEN PRINT PMT$(2):GOTO 2200
2250 IF ANY$="no" THEN 2450
2275 LOCATE 14,1: PRINT " When promoted, enter FIN. Enter number of units next"
2300 LOCATE 15,1:PRINT PMT$(6):LOCATE 15,1:
      INPUT " Enter FIN (from 1 to 41) here: ",NFRAG
2325 IF NFRAG<1 OR NFRAG>41 THEN PRINT " Input is out of range! Try again":
      GOTO 2300
2350 IF NFRAG<>INT(NFRAG) THEN PRINT " Integer input needed! Try again":
      GOTO 2300
2375 LOCATE 17,1:PRINT PMT$(6):LOCATE 17,1:INPUT " Enter number of specified
      fragments in molecule. ",NOF(NFRAG)
2400 IF NOF(NFRAG)<0 OR INT(NOF(NFRAG))<>NOF(NFRAG) THEN PRINT PMT$(2):GOTO 2375
2425 GOTO 1850
2450 SUMDP=0:SUMDV=0:SUMDT=0:MWT=0
2475 FOR J%=1 TO 41
2500 SUMDP=SUMDP+NOF(J%)*PON(J%):SUMDV=SUMDV+NOF(J%)*VON(J%)
2525 SUMDT=SUMDT+NOF(J%)*TON(J%):MWT=MWT+MOW(J%)*NOF(J%):NEXT J%
2550 THETA=.567+SUMDT-SUMDT^2
2575 LOCATE 14,1:PRINT PMT$(6):LOCATE 14,1:PRINT " Molecular Weight computed
      from your inputs = " MWT
2580 IF LIMIT(5)=0 THEN 2600 ELSE PRINT " Molecular Weight in File "
      PMT$(14)" = "PANV(91)
2585 PRINT " Other than round-off error, discrepancy may indicate error
      in inputs "
2590 PRINT " to the boiling point routine or in your input to the .DAT file. "
2600 PCRT=1/(.34+SUMDP)^2: VCRIT=40+SUMDV:FACT1=(1-THETA)^(2/7)
2625 BETA=(1.255+(FACT1-.048)*LOG(VCRIT)+FACT1*LOG(PCRT))/FACT1
2650 TCRIT=EXP(BETA)/82.054: TBOIL=THETA*TCRIT: ANSWER=TBOIL-273.2
2675 IF SLN=4 THEN RETURN ELSE LOCATE 20,1:PRINT PMT$(6):PRINT PMT$(6):
      LOCATE 20,1:GOSUB 15800
2700 RETURN

```

Figure A-8. Boiling Point Estimation Subroutine

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The CRT will display 41 different structure fragments in a table. You will be prompted to enter the identification number for a given fragment (FIN) of the subject pollutant and then the number of times that fragment occurs in the pollutant molecule. Your entry will be echoed back. You will be queried if you wish to do more. If you select yes, the table will re-display with the previous selection posted. This sequence is repeated until you respond 'no' to the 'Do you want to do more?' query.

In the table, there are coded abbreviations. 'NR' indicates a non-ring structure, 'RG' a ring. Rings can be either aliphatic or aromatic. Other abbreviations are alc=alcohol, phi=phenol, ald=aldehyde, est=ester. The triple bond (see FIN9 and FIN10) appears as '-#'. As examples of input, dinitrophenol would appear as 3FIN14 (=CH- in a ring), 3FIN15 (=C< in a ring), 1FIN22 (phenolic OH), and 2FIN37 (nitro groups). The compound DBCP 1,2-dibromo-3-chloropropane or CH2Br-CHBr-CH2Cl appear as 2FIN2 (-CH2- non-ring), 1FIN3 (-CH< non-ring), 2FIN19 (bromine), and 1FIN18 (chlorine). Entries need not be made in FIN order.

Enter 'yes' or 'no'.
Do you wish to continue analysis? yes

MILLER BOILING POINT METHOD FRAGMENTS ID TABLE			
OFIN1 -CH3 [NR]	OFIN2 -CH2- [NR]	OFIN3 -CH< [NR]	OFIN4 >C< [NR]
OFIN5 =CH2 [NR]	OFIN6 =CH- [NR]	OFIN7 =C< [NR]	OFIN8 =C= [NR]
OFIN9 -#CH [NR]	OFIN10 -#C- [NR]	OFIN11 -CH2- [RG]	OFIN12 -CH< [RG]
OFIN13 >C< [RG]	OFIN14 =CH- [RG]	OFIN15 =C< [RG]	OFIN16 =C= [RG]
OFIN17 -F	OFIN18 -Cl	OFIN19 -Br	OFIN20 -I
OFIN21 -OH alc	OFIN22 -OH phi	OFIN23 -O- [NR]	OFIN24 -O- [RG]
OFIN25 >C=O [NG]	OFIN26 >C=O [RG]	OFIN27 -CH=O ald	OFIN28 -COOH acid
OFIN29 -COO- est	OFIN30 =O other	OFIN31 -NH2	OFIN32 >NH [NR]
OFIN33 >NH [RG]	OFIN34 >N- [NR]	OFIN35 >N- [RG]	OFIN36 -CN
OFIN37 -NO2	OFIN38 -SH	OFIN39 -S- [NR]	OFIN40 -S- [RG]
OFIN41 =S			

When prompted, enter FIN. Enter number of units next
Enter FIN (from 1 to 41) here: 14

Enter number of specified fragments in molecule. 3

Figure A-9. Miller Boiling Point Method Displays: Information and Tableau.

(which is also Figure 14 in the main text) is displayed by lines 1850-2125.

At line 2150, ZIT% sums the number of fragments in the tableau. If ZIT% is zero, lines 2200-2250 are bypassed. At line 2275 through 2400, the entries for NFRAG, the number identifier for a given fragment, and NOF(NFRAG), the number of the given fragment in the molecule, are entered. The location of the tableau and these entries on the CRT screen is fixed (note use of the LOCATE command). At line 2425, control is sent back to line 1850, which again displays the tableau with the updated fragments listing. When ZIT% is not zero, the message at 2200 is displayed on line 20 of the screen (if ZIT% is zero, no entries have been made, and the program assumes you will make some). If you respond 'yes', control goes to line 2275. If you respond 'no', the sums of products NOF(J%)xPON(J%), NOF(J%)xVON(J%), NOF(J%)xTON(J%), and NOF(J%)xMOW(J%) are computed at lines 2500 and 2525 respectively as SUMDP, SUMDV, SUMDT, and MWT. At line 2575, the computed molecular weight, MWT, is displayed. Lines 2580-2590 is an advisory message concerning the value of

PANV(91) displayed when $\text{LIMIT}(5) = 1$. MWT should equal PANV(91), or differ slightly due to the number of significant figures used in molecular weight calculations. The mathematics continues to line 2650, where ANSWER is computed. Line 2675 has a conditional statement to return the boiling point subroutine to one of the vapor pressure methods (see Section A.8.5, "Mackay's Method #2"). Otherwise, the boiling point result is printed on the twentieth line of the monitor display.

A.8.4 The Water Solubility Estimation Subroutine

The code for this subroutine is found in Figure A-10. The information screen is in WATERSOL.CMP (line 775). The selection menu is displayed by lines 825 to 1000. Line 1030 calls the short subroutine at line 15750, which provides the numerical value for the variable LKOW. Since equation 2.3 ($\text{SLN} = 2$) requires no other inputs, line 1075 directs its evaluation at line 1175. The other equations require molecular weight input (the variable MWT); hence the subroutine at line 15775 is called by line 1075.

Line 1075 concludes with an "ON SLN+1 GOTO..." branch command. Actually, two of the five options have been disposed of; this statement addresses the other three. Line 1200 sets $\text{TMELT} = 25$ so that the equation at line 1275 can be used for the $\text{SLN} = 3$ option. Line 1225 requests a melting point for the $\text{SLN} = 4$ option. Line 1250 resets TMELT to 25 if a smaller value is entered at line 1225. Then line 1275 processes both options.

A.8.5 The Vapor Pressure Estimation Subroutine

The code is in Figure A.11. VAPRESS.CMP, the file for the vapor pressure information screen is downloaded and displayed, followed by VAPMENU.CMP, which contains the options menu. At line 2875, you enter TCAL, the temperature at which the vapor pressure is to be estimated; it is then converted to $^{\circ}\text{K}$ as TCALK. STAT\$ is provided to assess the state of the substance at TCAL; it is initially "no" (substance is a solid). Line 2900 directs execution to the start of each calculation option.

Mackay's method 1 ($\text{SLN} = 1$) starts at line 2925. If entry to CHMPRP11 is from CHMFIL11, the line 2925 transfers PANV(92) and PANV(93) to the variables TM and TB. Otherwise, at lines 2950-2975, you provide these values. At line 3050, RTM, the ratio of the melting point temperature to the calculation temperature ($^{\circ}\text{K}$), is compared to one. If $\text{RTM} < 1$, the substance is a liquid and at line 3050, $\text{FACTOR} = 0$. Otherwise, FACTOR is valued as $6.8 \times (\text{RTM} - 1)$. At line 3075, the variable LNPVA, in units of natural log pressure (atmospheres), is computed. Line 3100 computes ANSWER in mm Hg from LNPVA.

Watson's method ($\text{SLN} = 2$) starts at line 3150. Part of this routine is executed when you select option "5", so PREF is pre-set to 760 mm Hg. At line 3160, the boiling point temperature (TREF) is valued. At line 3170, if $\text{LIMIT}(5) = 1$, PANV(92) is compared to TCAL. If PANV(92) exceeds TCAL, the substance is a liquid, and STAT\$ is reset to "yes". If $\text{LIMIT}(5) = 0$, execution skips to line 3200, where STAT\$ is manually entered. At lines 3250-3305, a message is displayed about the next information screen table,

```

775 PNTR=95:BLURB$(21)="watersol.cmp":SK=0:GOSUB 15400
825 CLS:PRINT " ***** WATER SOLUBILITY ESTIMATION MENU *****"
850 PRINT TAB(5) "Enter value for desired estimation method"
875 PRINT TAB(5) "Select '0' to exit without any estimate performed"
900 PRINT TAB(5) "Select '1' for LRR equation 2.2 (also need MW)"
925 PRINT TAB(5) "Select '2' for LRR equation 2.3"
950 PRINT TAB(5) "Select '3' for LRR equation 2.15 (also need MW)"
975 PRINT TAB(5) "Select '4' for LRR equation 2.15 with melt pt. correction"
1000 INPUT " (need MW and Tmelt). Enter selection here: ",SLN
1025 IF SLN <0 OR SLN >5 OR SLN <> INT(SLN) THEN PRINT PMT$(2):GOSUB 15850:
      GOTO 825
1030 IF SLN=0 THEN 1325 ELSE GOSUB 15750
1075 IF SLN=2 THEN 1175 ELSE GOSUB 15775:ON SLN+1 GOTO 1325,1150,1175,1200,1225
1150 SWMUMW=10^(-1.37*LKOW+7.26):ANSWER=SWMUMW*MWT/1000:GOTO 1300
1175 ANSWER=10^(-.922*LKOW+4.184):GOTO 1300
1200 TMELT=25:GOTO 1275
1225 IF LIMIT(5)=0 THEN INPUT " Enter melting point, deg C: ",TMELT
      ELSE TMELT=PANV(92):PRINT PANM$(92) " = " PANV(92)
1250 IF TMELT<25 THEN TMELT=25
1275 MPSWM=10^(1.339*LKOW-.978+.0095*(TMELT-25)):SWM=1/MPSWM:
      ANSWER=SWM*MWT*1000
1300 GOSUB 15800
1325 RETURN

```

Figure A-10. Water Solubility Estimation Subroutine

(Figure 16, main text). After a pause at line 3325, the subroutine starting at line 4250 is called. First, data are down-loaded from VPFACTOR.CMP to the 35 elements in the array KF. Line 4325 provides the information to down-load the information screen file VPTABLE.CMP, whose display appears in Figure 16 of the main text. At line 4350, you provide the value to KFINDEX, the structure identification index. Then at line 4425, the element KF(KFINDEX) is called KFCAL. Then execution passes back to line 3325 to value TREFK and TEQB.

At lines 3375-3450, the exponent MEX is computed. If STAT\$ = "yes" (the substance is a liquid at room temperature), MEX = 0.19. Otherwise, the value of MEX depends upon TEQM. At line 3390, TEQM is equated to TEQB for SLN = 2 (the other part of this command is needed for the SLN = 5 option). At line 3475, the intermediate variable FA1416 is calculated. When SLN = 2, the term $\log(\text{PREF}/760)$ is zero, and the calculation at line 3550 for LNPVA corresponds to equation 14-16 in Lyman et al.⁶ The input data for the estimate are displayed at lines 3580-3590. Execution passes to line 3100 to convert LNPVA to pressure in mm Hg and display this pressure as ANSWER.

The interpolation method (SLN = 3) starts at line 3625. The two sets of temperature and pressure data are entered at lines 3675-3750. At line 3925, the variable RSL is entered, which governs if a solid phase adjustment to a liquid vapor pressure estimate is needed. At line 4000, the slope (ASLOPE) and the intercept (BINT) are computed for the linear relation. If RSL <> 2, LNPVA is computed at line 4025 and control passes to line 3100. If RSL = 2, the solid vapor pressure adjustment (FACTOR, the same as at line 3050) is made at line 4075.

Mackay's method 2 (SLN = 4) starts at line 4100. Here, the boiling point is estimated from the melting point. Control is first passed to line 1650 in a GOSUB call. This enters the boiling point estimation routine, described in Figure A-8, and uses the equation at line 1675. Line 2675 in that routine

```

2725 PMTR=96:BLURB$(21)="vapress.cmp":SK=0:GOSUB 15400
2775 CLS:BLURB$(21)="vapmenu.cmp":SK=1:GOSUB 15550
2800 INPUT " Enter your selection (from 0 to 5): ",SLN
2825 IF SLN<0 OR SLN>5 OR SLN<>INT(SLN) THEN PRINT PMT$(2):GOTO 2775
2850 IF SLN<>INT(SLN) THEN PRINT PMT$(2):GOTO 2775
2860 IF SLN=0 THEN GOTO 4475
2875 INPUT " Enter temperature in DegC for calculation result: ",
      TCAL:TCAL=TCAL+273.2:STAT$="no"
2900 ON SLN GOTO 2925,3150,3625,4100,4150
2925 IF LIMIT(5)=0 THEN 2950 ELSE TM=PANV(92):TB=PANV(93)
2930 PRINT PANM$(92) " = " PANV(92):PRINT PANM$(93) " = " PANV(93):GOTO 3025
2950 INPUT " Enter melting point in Deg C: ",TM
2975 INPUT " Enter boiling point in Deg C: ",TB
3000 IF TM>TB THEN PRINT " Entries are probably reversed! Try again.":GOTO 2950
3025 TM=TM+273.2:TB=TB+273.2:RTB=TB/TCAL:RTM=TM/TCAL
3050 IF RTM<1 THEN FACTOR=0 ELSE FACTOR=6.8*(RTM-1)
3075 LNPVA=-(4.4+LOG(TBK))*(1.803*(RTB-1)-.803*LOG(RTB))-FACTOR
3100 ANSWER=760*EXP(LNPVA)
3125 GOSUB 15800:GOTO 4475
3150 PREF=760
3160 IF LIMIT(5)=0 THEN INPUT " Enter boiling point in DegC: ",TREF:GOTO 3200
      ELSE TREF=PANV(93)
3170 IF LIMIT(5)=1 THEN IF PANV(92)<TCAL THEN STAT$="yes":GOTO 3250
3180 IF LIMIT(5)=1 THEN GOTO 3250
3200 PRINT PMT$(1):INPUT " Is substance a liquid at calculation temp? ",STAT$
3225 IF STAT$<>"yes" AND STAT$<>"no" THEN PRINT PMT$(2):GOTO 3200
3250 PRINT " You will be shown a table of general compound groups. Choose the"
3275 PRINT " number of the group describing your compound. Note, for mixed"
3300 PRINT " aromatic constituents, -OH takes precedence. For simple aromatics"
3305 PRINT " consider the phenyl group as a n-Alkane (selection #1)."
3325 SK=0:GOSUB 15675:GOSUB 4250:TREFK=TREF+273.2:TEQB=TCAL/TREFK
3375 IF STAT$="yes" THEN MEX=.19:GOTO 3475
3390 IF SLN=5 THEN DECP=(1/2.303)*LOG(760/PREF):TEQM=TCAL/(TREFK+64*DECP)
      ELSE TEQM=TEQB
3400 IF TEQM>.6 THEN MEX=.36:GOTO 3475
3425 IF TEQM<.5 THEN MEX=1.19:GOTO 3475
3450 MEX=.8
3475 FA1416=KFCAL*(8.75+1.987*(LOG(TREFK)-LOG(PREF/760)))
3500 COEF=FA1416/(.97*1.987):TERM=3-2*TEQB
3550 LNPVA=COEF*(1-(1/TEQB)*(TERM*MEX)-2*MEX*(LOG(TEQB))*TERM*(MEX-1))
3575 IF SLN=5 THEN LNPVA=LNPVA+LOG(PREF/760)
3580 IF SLN=2 THEN PRINT " Boiling Point (C) = "TREF TAB(35)
      ELSE PRINT " Ref Pressure(mm Hg) = "PREF " at Ref Temperature(C) = "TREF
3590 IF STAT$="yes" THEN PRINT " Ambient state of substance is liquid"
      ELSE PRINT " Ambient state of substance is solid"
3600 GOTO 3100
3625 PRINT " Extrapolation method uses two Temp-VP datum and assumes"
3650 PRINT " that Ln(VP) proportional to 1/T degK inside and beyond range."
3675 PRINT " Inputs for the Lower temperature in range.":
      INPUT " Enter low range temp, DegC: ",T1C
3700 INPUT " Enter low range VP in mm Hg: ",P1
3725 PRINT " Inputs for Higher temperature in range.":INPUT " Enter high
      range temp, DegC: ",T2C
3750 INPUT " Enter high range VP in mm HG: ",P2
3775 IF P2<P1 THEN PRINT " Pressure at high temp lower than at low temp!
      Try again":GOTO 3675
3800 IF T1C>T2C THEN PRINT " Temperatures in wrong order! Try again.":GOTO 3675
3825 PRINT " Enter the value from 1 to 3 which best describes your situation"
3850 PRINT " Enter '1' if substance is liquid at calc. temp & in range"
3875 PRINT " Enter '2' if substance is solid at calc. temp & liquid in range"
3900 PRINT " Enter '3' if substance is solid at calc. temp & solid in range"

```

Figure A-11. Vapor Pressure Estimation Subroutine (page 1 of 2 pages)

A11

```

3925 INPUT " Enter your value (1, 2, or 3 ) : ",RSL
3950 IF RSL<>1 AND RSL<>2 AND RSL<>3 THEN PRINT PMT$(2):GOTO 3825
3975 Y1=LOG(P1/760):Y2=LOG(P2/760):X1=1/(T1C+273.2):X2=1/(T2C+273.2)
4000 ASLOPE=(Y2-Y1)/(X2-X1):BINT=Y1-ASLOPE*X1
4025 IF RSL=1 OR RSL=3 THEN LNPVA=ASLOPE*1/TCAL+BINT:GOTO 3100
4050 IF LIMIT(5)=1 THEN TM=PAV(92):PRINT PAVM$(92) " = " PAV(92)
      ELSE INPUT " Enter melting point in degC: ",TM
4075 TMK=TM+273.2:RTM=TMK/TCAL:FACTOR=6.8*(RTM-1):
      LNPVA=ASLOPE*1/TCAL+BINT-FACTOR:GOTO 3100
4100 GOSUB 1650:TM=MELT:TB=ANSWER:GOTO 3025
4150 INPUT " Enter reference temperature for reduced pressure: ",TREF
4175 INPUT " Enter VP at reference temperature: ",PREF
4200 GOTO 3170
.....Subroutine to down-load and select Watson's KF Factor.....
4250 OPEN "VPFACTOR.CMP" FOR INPUT AS #1
4275 FOR J%=1 TO 35:INPUT #1,KF(J%):NEXT J%:CLOSE #1
4325 CLS:BLURB$(21)="vptable.cmp":SK=1:GOSUB 15550
4350 INPUT " Enter identification number: ",KFINDEX
4375 IF INT(KFINDEX)<>KFINDEX THEN PRINT " Non-Integer Entry!! Try Again":
      GOTO 4325
4400 IF KFINDEX<1 OR KFINDEX>35 THEN PRINT " Entry must be in range 1-35!!
      Try Again":GOTO 4325
4425 KFCAL=KF(KFINDEX):PRINT " KFCAL= " KF(KFINDEX):RETURN
4475 PRINT " VP computed for Deg C Temp of "TCAL:RETURN

```

Figure A-11. Vapor Pressure Estimation Subroutine (page 2 of 2 pages)

causes the boiling point printout to be bypassed, as the SLN = 4 condition refers to this method and the return is to line 4100. At this point, MELT (the variable used at line 1650 to represent the melting point) is equated to TM. ANSWER (which at this point contains the estimated boiling point) is equated to TB. Then control is passed to line 3025, where the SLN = 1 execution train carries out the remainder of the calculations.

Watson's reduced pressure method (SLN = 5) requests input of TREF and PREF at lines 4150 and 4175, respectively. Then control passes to line 3170, which is in the SLN = 2 routine. At line 3390, an adjustment is made to TEQM if STAT\$ = "no". This heuristic adjustment is needed because MEX is a function of the boiling point. The adjustment is based on my study of temperature - vapor pressure data for the liquid state of several organic substances that are solids at room temperature. For vapor pressures in the range of 1 to 400 mm Hg, there is a temperature increase of about 64 °C for each magnitude increase in vapor pressure. TEQM can be thought of as a "pseudo" boiling point. At line 3475, the calculation of variable FA1416 corresponds to equation 14-24 in Lyman et al.⁶. At line 3575, the correction factor for the reduced pressure is included in the LNPVA calculation.

A.8.6 The Koc Estimation Subroutine

The code for this subroutine is in Figure A-12. The options presented are on the information screen down-loaded from KOCINFO.CMP (line 5025). SLN is entered at line 5050. Options 1-3 deal with log Kow correlations and are accessed at line 5125; ANSWER is valued at line 5175, 5200 or 5225, respectively. Then control is passed to line 5410, which displays ANSWER for all calculation options.

For water solubility-based correlations, WSOL is supplied by the first GOSUB call at line 5250. Options other than SLN = 7 require molecular weight

```

5025 PNTR=101:BLURB$(21)="kocinfo.cmp":SK=1:GOSUB 15400
5050 INPUT " Enter your selection (from 0 to 7): ",SLN:IF SLN=0 THEN 5425
5075 IF SLN >7 OR SLN<0 OR INT(SLN)<>SLN THEN PRINT PMT$(2):
      GOSUB 15850:GOTO 5025
5100 IF SLN>3 THEN 5250 'leave water solubility stuff for later
5125 GOSUB 15750: ON SLN GOTO 5175,5200,5225
5175 ANSWER=10^(.806*LKOW+.473):GOTO 5410
5200 ANSWER=10^(.881*LKOW+.214):GOTO 5410
5225 ANSWER=10^(.533*LKOW+1.151):GOTO 5410
5250 GOSUB 15825:IF SLN=7 THEN ANSWER=10^(-.55*(1/2.303)*LOG(WSOL)+3.64):
      GOTO 5410 ELSE GOSUB 15775
5325 LWS=(1/2.303)*LOG(WSOL/(1000*MWT)):ON SLN-3 GOTO 5350,5375,5400
5350 ANSWER=10^(-.602*LWS+.656):GOTO 5410
5375 ANSWER=10^(-.641*LWS+.53):GOTO 5410
5400 ANSWER=10^(-.45*LWS+1.05)
5410 GOSUB 15800
5425 RETURN
.....Subroutine for Ksp and Ksv.....
5450 PNTR=102
5475 BLURB$(21)="kspksv.cmp":CLS:SK=1:GOSUB 15500
5500 PRINT "***** KSV OR KSP ESTIMATION MENU *****"
5525 PRINT " Select '0' to exit without any estimate performed."
5550 INPUT " Select '1' to do Travis and Arms correlation: ",SLN
5575 IF SLN=0 THEN 5700
5600 IF SLN <> 1 THEN PRINT PMT$(2):GOTO 5500
5625 GOSUB 15750:ANSWER=10^(1.558-.578*LKOW):GOSUB 15800
5700 RETURN
5725 PNTR=103:GOTO 5475

```

Figure A-12. Koc, Ksv, and Ksp Estimation Subroutines.

input. Then, the equation corresponding to $SLN = 7$ provides that option's ANSWER. Otherwise, the subroutine to supply MWT is called. At line 5325, the \log_{10} of molar solubility, LWS, is computed and control is passed to line 5350, 5375, or 5400, depending upon whether SLN is 4, 5 or 6, respectively.

A.8.7 The Ksp and Ksv Estimation Subroutine

The code for this short subroutine (one calculation option) is also shown in Figure A-12. If Ksp is the prediction variable, the subroutine starts at line 5450. Otherwise, the subroutine starts at line 5725. From line 5475, both variables are processed identically. Line 5625 issues the call to obtain value of $\log Kow$, LKOW, which is used to evaluate ANSWER at that line.

A.8.8 The BCF Estimation Subroutine

The code for this subroutine is at the top of Figure A-13. Input of $\log Kow$ is effected at line 6075 to solve the equation

$$BCF = 10(0.76 \times \log Kow - 0.23).$$

Similarly, water solubility (WSOL) input and evaluation of ANSWER occurs at line 6125. Koc (KOC) is input at line 6175; the equation solved is at line 6200. In lines 6125 and 6200, LWSOL and LKOC are base ten logarithms; the "log" function in GWBASIC is in terms of base e.


```

.....The BCF Estimation Subroutine
5975 PNTR=111:BLURB$(21)="bcfinfo.cmp":SK=1:GOSUB 15400
6000 INPUT "Enter your selection: ",SLN
6025 IF SLN <0 OR SLN>4 OR SLN<>INT(SLN) THEN
PRINT "Entry out of range":GOTO 5975
6050 ON SLN+1 GOTO 6250,6075,6125,6175
6075 GOSUB 15750:ANSWER=10^(1.76*LKOW-.23):GOTO 6225
6125 GOSUB 15825:LWSOL=(1/2.303)*LOG(WSOL):ANSWER=10^(2.791-.564*LWSOL):
GOTO 6225
6175 IF LIMIT(5)=0 THEN INPUT "Enter Koc Value (L/kg): ",KOC.
ELSE KOC=PANV(101):PRINT PANM$(101) " = "PANV(101)
6200 LKOC=(1/2.303)*LOG(KOC):ANSWER=10^(1.119*LKOC-1.579):GOTO 6225
6225 GOSUB 15800
6250 RETURN
..... The Kvw and Kwp Estimation Subroutines.....
6275 PNTR=112
6300 BLURB$(21)="kwpvinfo.cmp":CLS:SK=0:GOSUB 15500
6325 PRINT "***** SELECTION MENU FOR KVV AND KWP *****"
6350 PRINT "Select '0' to exit without any estimate performed"
6375 PRINT "Select '1' to do Briggs' equation"
6400 PRINT "Select '2' to compute based on Ksv"
6425 PRINT "Select '3' to compute based on Ksp"
6450 PRINT "Select '4' to set Kvp equal to Kvv (CHMFIL11 entry only)"
6475 INPUT "Enter your selection value here: ",SLN
6500 IF LIMIT(5)=0 AND SLN=4 THEN PRINT "Sorry, can't do in the off-line
mode.":GOTO 6325
6525 IF SLN <0 OR SLN>4 THEN PRINT PMT$(2):GOTO 6325
6550 IF SLN<>INT (SLN) THEN PRINT PMT$(2):GOTO 6325
6575 IF SLN=0 THEN 6599 ELSE ON SLN GOSUB 6600,6675,6775,6850
6580 IF SLN=6 THEN 6325 ELSE GOSUB 15800
6599 RETURN
6600 GOSUB 15750:E1=.95*LKOW-2.05:E2=-.178*(LKOW-1.78)^2:
ANSWER=5*(.82+10^E1)*(10^E2):RETURN
6675 IF LIMIT(5)=0 THEN INPUT "Enter Ksv: ",KSV ELSE
KSV=PANV(103):PRINT PANM$(103) " = "PANV(103)
6700 IF LIMIT(5)=0 THEN INPUT "Enter reference foc: ",FOCR
ELSE FOCR=PANV(105):PRINT PANM$(105) " = "PANV(105)
6725 IF LIMIT(5)=0 THEN INPUT "Enter Koc: ",KOCR
ELSE KOCR=PANV(101):PRINT PANM$(101) " = "PANV(101)
6750 ANSWER=KSV*(FOCR*KOCR):RETURN
6775 IF LIMIT(5)=0 THEN INPUT "Enter Ksp: ",KSP
ELSE KSP=PANV(102):PRINT PANM$(102) " = "PANV(102)
6800 IF LIMIT(5)=0 THEN INPUT "Enter reference foc: ",FOCR
ELSE FOCR=PANV(104):PRINT PANM$(104) " = "PANV(104)
6825 GOTO 6725
6850 IF LIMIT(6)=23 THEN ANSWER=PANV(112):RETURN
6875 PRINT "Sorry, can't set Kvp = Kwp. Jot down value of Kvp ":
PRINT "you want to use and insert it in Kvp in another pass
through CHMFIL11.":SLN=6:RETURN
6950 PNTR=113:GOTO 6300

```

Figure A-13. BCF, Kvw, and Kwp Estimation Subroutines.

A.8.9 The Kvw and Kwp Estimation Subroutine

The code for this subroutine is also in Figure A-13. If entry is at line 6275, PNTR = 112. Otherwise, entry is at line 6950, and PNTR = 113. Line 6600 first obtains log Kow and then computes ANSWER for the first option. Options 2 and 3 are based on the products Ksv x Koc x foc and Ksp x Koc x foc respectively as estimators for Kvw and Kwp. For option 2, Ksv, foc, and Koc are obtained at lines 6675, 6700, and 6725, respectively. For option 3, Ksp is entered at line 6775, but internally is still called KSV. The foc corresponding to Ksp is entered at line 6800. Then line 6725 is entered to obtain Koc, after which ANSWER is computed at line 6750.

Option 4 applies only to entry from CHMFIL11. If this option is selected after entry from OPEN 11, line 6500 will detect this, and route you back to the selection menu. The option 4 algorithm is at line 6850. LIMIT(6) = 23

corresponds to entry from the Kwp routine in CHMFIL11. In this case, the algorithm replaces the value of element PANV(113) with PANV(112).

A.8.10 The Kpat Estimation Subroutine

The code for this short subroutine is in Figure A-14, and includes two estimation methods. The first is at line 4825, where log Kow is input (LKOW), the second is at line 4875, where water solubility (WSOL) is input.

A.8.11 The Kpm Estimation Subroutine

The code for this subroutine is in Figure A-15. Lines 7000-7200 display the selection menu with six available computation options. The first three options use fm (called FATMEAT). Default values of fm and fd (called FATMILK) are pre-set at line 7260. The "ON SLN GOTO..." command at line 7275 directs the computation for the given option.

Option 1 uses the default value of FATMEAT and the value of KPAT supplied at line 7325. ANSWER is computed for options 1 through 3 at line 7350 and displayed by line 7280. Line 7290 is a common RETURN to exit from all options. Option 2 starts at line 7400. The GOSUB call to line 15000 causes .LDS files to be displayed. The selected file to be down-loaded is input at line 15100. After checks for proper file-name, the designated file is down-loaded at line 15250 into the first 90 elements of the PANV array. The filename is loaded into PMT\$(12) at line 15310. Thus, the down-loaded data are in an on-line stored status. The return from this subroutine is to line 7425. Here, if PANV(42) = 0, a message is displayed, and control passes back to the selection menu. This avoids a potentially fatal "division by zero" error. At line 7485, the down-loaded values of fm and fd are shown. If undesired, you can return to the selection menu.

At line 7500, FATMEAT is valued, and control passes to line 7325. Option 3 starts at line 7425 (in option 2, a .LDS file was immediately down-loaded; here, whatever is in on-line storage is accessed). The subsequent steps are described above.

Option 4 starts at line 7525, where the value of KPD is obtained. ANSWER is computed at line 7550 for options 4 through 6. Option 5 follows option 2 through line 7500. There, when SLN = 5, line 7600 is accessed, where FATMEAT and FATMILK are evaluated. Then line 7525 is accessed, where the procedure for option 4 is joined. Option 6 follows option 3 to line 7500 and then skips over to line 7600, at which execution is identical to that for option 5.

A.8.12 The Kpd Estimation Subroutine

This subroutine's code is in Figure A-16, and mirrors that of the Kpm subroutine, replacing Kpd with Kpm, fm with fd, and vice versa. FATMEAT and FATMILK are initially valued at line 8050. Option 1 uses the KPAT from line 8075 and the default FATMILK to compute ANSWER at line 8100. In option 2, the subroutine at line 15000 (see Figure A-16) is entered to download a .LDS file. The return is to lines 8175. Here, if PANV(41) = 0, a message is displayed, and control passes back to the selection menu to avoid a

```

4525 PNTR=106:BLURB$(21)="kpatinfo.cmp":SK=0:GOSUB 15400
4550 PRINT " ***** Kpat ESTIMATION MENU *****:PRINT
4575 PRINT " Two correlations are presented here, which were suggested by"
4600 PRINT " Garten and Trebalka: ES&T 17(10):590-595(1983). They are"
4625 PRINT " considered to be more robust than earlier relations suggested"
4650 PRINT " by Kenaga ES&T 14(5):553-556(1980)."
4675 PRINT:PRINT " Select '0' for exit without any estimation performed."
4700 PRINT " Select '1' for G&T Log Kow correlation."
4725 PRINT " Select '2' for G&T Water solubility correlation."
4750 INPUT " Enter your selection here: ",SLN
4775 IF SLN<>0 AND SLN<>1 AND SLN<>2 THEN PRINT PMT$(2):GOTO 4550
4800 ON SLN+1 GOTO 4950,4825,4875
4825 GOSUB 15750:ANSWER=10*(-3.935+.511*LKOW):GOTO 4925
4875 GOSUB 15825:ANSWER=10*(-1.633-.608*(1/2.303)*LOG(WSOL))
4925 GOSUB 15800
4950 RETURN

```

Figure A-14. Kpat Estimation Subroutine

```

6975 PNTR=114:BLURB$(21)="kpminfo.cmp":SK=0:GOSUB 15400
7000 PRINT " ***** Kpm ESTIMATION MENU *****
7025 PRINT:PRINT " Enter value for desired function"
7050 PRINT " Select '0' to exit without any calculation"
7075 PRINT " Select '1' to estimate Kpm from Kpat and DEFAULT fm data"
7100 PRINT " Select '2' to estimate Kpm from Kpat and .LDS file fm data"
7125 PRINT " Select '3' to estimate Kpm from Kpat and on-line fm data"
7150 PRINT " Select '4' to estimate Kpm from Kpd with DEFAULT fm/fd data"
7175 PRINT " Select '5' to estimate Kpm from Kpd with .LDS file fm/fd data"
7200 PRINT " Select '6' to estimate Kpm from Kpd with on-line fm/fd data"
7225 INPUT " Enter your selection: ",SLN
7250 IF INT(SLN)<>SLN OR SLN<0 OR SLN>6 THEN PRINT PMT$(2):GOTO 7000
7260 FATMEAT=.25:FATMILK=.04
7275 IF SLN=0 THEN 7290 ELSE ON SLN GOTO 7325,7400,7425,7525,7400,7425
7280 GOSUB 15800
7290 RETURN
7325 IF LIMIT(5)=0 THEN INPUT " Enter Kpat Value: ",KPAT
      ELSE KPAT=PANV(106):PRINT PANM$(106) " = " PANV(106)
7330 PRINT " The fraction of fat in meat is " FATMEAT
7350 ANSWER=KPAT*FATMEAT:GOTO 7280
7400 GOSUB 15000
7425 IF PANV(42)<>0 THEN GOTO 7485 ELSE PRINT " You don't have a valid
      data set! Last .LDS file was: "PMT$(12)
7450 PRINT " If no file shown, no on-line data exist. If a file is shown,
      fm or fd":PRINT " is still zero. Try another method and check file.":
      GOTO 7000
7485 PRINT " The current values of fm and fd are "PANV(41) " and "PANV(42)
7488 INPUT " Do you wish to continue with on-line info?: ",AN$
7490 IF AN$="no" THEN GOTO 7000
7495 IF AN$<>"yes" AND AN$<>"no" THEN PRINT PMT$(2):GOTO 7485
7500 IF SLN=2 OR SLN=3 THEN FATMEAT=PANV(41):GOTO 7325 ELSE GOTO 7600
7525 IF LIMIT(5)=0 THEN INPUT " Enter Kpd Value: ",KPD
      ELSE KPD=PANV(115):PRINT PANM$(115) " = " PANV(115)
7530 PRINT " The fraction of fat in milk is " FATMILK
7535 PRINT " The fraction of fat in meat is " FATMEAT
7550 ANSWER=KPD*FATMEAT/FATMILK:GOTO 7280
7600 FATMEAT=PANV(41):FATMILK=PANV(42):GOTO 7525
.....Subroutine to down-load .LDS file.....
15000 PRINT " REVIEW OF .LDS FILES AVAILABLE ":FILES PMT$(5)+".lds"
15100 INPUT " ENTER .LDS FILE (including .lds extension): ",FIL$
15150 IF LEN(FIL$)>12 THEN PRINT " Name too long!! Try again":GOTO 15100
15200 IF RIGHT$(FIL$,4)<>".lds" THEN PRINT " Wrong file type!! Try again":
      GOTO 15100
15250 OPEN PMT$(5)+FIL$ FOR INPUT AS #1:FOR J%=1 TO 90:
      INPUT #1,PANV(J%):NEXT J%:CLOSE #1
15300 PRINT " Downloading of "FIL$ " completed."
15310 PMT$(12)=PMT$(5)+FIL$:LIMIT(3)=10:LIMIT(4)=LIMIT(4) OR LIMIT(3):RETURN

```

Figure A-15. Kpm Estimation Subroutine

```

7725 PNTR=115:BLURB$(21)="kpdinfo.cmp":SK=0:GOSUB 15400
7750 PRINT " ***** Kpd ESTIMATION MENU *****"
7775 PRINT:PRINT " Enter value for desired function"
7800 PRINT " Select '0' to exit without any calculation"
7825 PRINT " Select '1' to estimate Kpd from Kpat and DEFAULT fd data"
7850 PRINT " Select '2' to estimate Kpd from Kpat and .LDS file fd data"
7875 PRINT " Select '3' to estimate Kpd from Kpat and on-line fd data"
7900 PRINT " Select '4' to estimate Kpd from Kpm with DEFAULT fm/fd data"
7925 PRINT " Select '5' to estimate Kpd from Kpm with .LDS file fm/fd data"
7950 PRINT " Select '6' to estimate Kpd from Kpm with on-line fm/fd data"
7975 INPUT " Enter your selection: ",SLN
8000 IF INT(SLN)<>SLN OR SLN<0 OR SLN>6 THEN PRINT PMT$(2):GOTO 7750
8050 FATMEAT=.25:FATMILK=.04
8060 IF SLN=0 THEN 8140 ELSE ON SLN GOTO 8075,8150,8175,8260,8150,8175
8075 IF LIMIT(5)=0 THEN INPUT " Enter Kpat Value: ",KPAT
    ELSE KPAT=PANV(106):PRINT PANM$(106) " = " PANV(106)
8080 PRINT " The fraction of fat in milk is "FATMILK
8100 ANSWER=KPAT*FATMILK
8125 GOSUB 15800
8140 RETURN
8150 GOSUB 15000
8175 IF PANV(41)<>0 THEN GOTO 8235 ELSE PRINT " You don't have a valid
    data set! Last .LDS file was: "PMT$(12)
8200 PRINT " If no file shown, no on-line data exist. If a file is shown,
    fm or fd":PRINT " is still zero. Try another method and check file.":
    GOTO 7750
8235 PRINT " The current values of fm and fd are " PANV(41) " and " PANV(42)
8240 INPUT " Do you wish to continue with on-line info?: ",ANS:
    IF ANS="no" THEN GOTO 7750
8245 IF ANS<>"yes" AND ANS<>"no" THEN PRINT PMT$(2):GOTO 8235
8250 IF SLN=2 OR SLN=3 THEN FATMILK=PANV(42):GOTO 8075 ELSE GOTO 8325
8260 IF LIMIT(5)=0 THEN INPUT " Enter Kpm Value: ",KPM
    ELSE KPM=PANV(114):PRINT PANM$(114) " = " PANV(114)
8280 PRINT " The fraction of fat in milk is " FATMILK:
    PRINT " The fraction of fat in meat is " FATMEAT
8300 ANSWER=KPM*FATMILK/FATMEAT:GOTO 8125
8325 FATMEAT=PANV(41):FATMILK=PANV(42):GOTO 8260

```

Figure A-16. Kpd Estimation Subroutine

potentially fatal "division by zero" error. Otherwise, the values of fm and fd are shown at line 8235. If you continue, FATMILK is valued at line 8250, and control passes back to line 8075. In option 3, execution starts at line 8175, and then follows that of option 2.

Option 4 starts at line 8260, where KPM is valued. The default FATMEAT and FATMILK are used to compute ANSWER, which is calculated at line 8300. Option 5 follows the option 2 algorithm through line 8250, where control passes to line 8325 to value FATMEAT and FATMILK. Option 6 follows the option 3 algorithm through line 8250, where control also transfers to line 8325.

A.8.13 The Kh Estimation Subroutine

The code for this subroutine is shown in Figure A-17. Here, Kh is computed as the ratio of vapor pressure to aqueous solubility, adjusted for input units, and expressed in dimensionless form. Line 8650 asks if the calculation is at 25 °C. If you respond "no", line 8725 requests a different temperature. Otherwise, 25°C is assumed. At line 8750, molecular weight data is obtained.

The next command picks up water solubility data from PANV(95) if you entered CHMPRP11 from CHMFIL11, and if so, transfers execution to line 8975. If you entered CHMPRP11 from OPEN11, you have the option to enter solubility in mg/L.

```

8450 PNTR=116:BLURB$(21)="henry.cmp":SK=0:GOSUB 15400
8475 PRINT " ***** Kh ESTIMATION MENU *****"
8525 PRINT " Select '0' to exit without any calculation."
8550 PRINT " Select '1' to compute Kh"
8575 INPUT " Enter your selection: ",SLN
8600 IF SLN=0 THEN GOTO 9250
8625 IF SLN<>1 THEN PMT$(2):GOTO 8500
8650 PRINT PMT$(1):INPUT " Is temperature of calculation 25C (298.2K)?: ",ANY$
8675 IF ANY$<>"yes" AND ANY$<>"no" THEN PRINT PMT$(2):GOTO 8650
8700 TEMP=298.2:IF ANY$="yes" THEN 8750
8725 INPUT " Enter temperature in degC here: ",TEMP:TEMP=TEMP+298.2
8750 GOSUB 15775:IF LIMIT(5)=1 THEN WSOL=PANV(95):PRINT PANM$(95) = "WSOL:
      GOTO 8975
8800 PRINT:PRINT " Water solubility units for input. Enter '1' for mg/L units,"
8825 INPUT " '2' for mole/L units, '3' for millimole/L units: ",UNO
8850 IF UNO<>1 AND UNO<>2 AND UNO<>3 THEN PMT$(2):GOTO 8800
8875 INPUT " Enter solubility limit in specified units: ",WSOL
8900 ON UNO GOTO 8975,8925,8950
8925 WSOL=WSOL*MWT*1000:GOTO 8975
8950 WSOL=WSOL*MWT
8975 IF LIMIT(5)=1 THEN VP=PANV(96):PRINT PANM$(96) = " VP:GOTO 9200
9000 PRINT:PRINT " Vapor pressure units for input. Enter '1' for torr(mm Hg)
      units"
9025 PRINT " Enter '2' for atmosphere units, enter '3' for Pascal units"
9050 INPUT " Enter code for units: ",UNO
9075 IF UNO<>1 AND UNO<>2 AND UNO<>3 THEN 9000
9100 INPUT " Enter saturation vapor pressure in specified units: ",VP
9125 ON UNO GOTO 9200,9150,9175
9150 VP=VP*760:GOTO 9200
9175 VP=VP/133.3
9200 ANSWER=(16.03*VP)/(TEMP*(WSOL/MWT))
9225 GOSUB 15800
9250 RETURN

```

Figure A-17. Kh Estimation Subroutine

mole/L, or millimole/L. The unit is entered (UNO, line 8825), followed by the numerical value (WSOL, line 8875). Based on the unit selection, WSOL is converted to a mg/L basis (lines 8925-8950). Line 8975 set VP = PANV(96) if LIMIT(5) = 1. Otherwise, manual entry of VP is required. First, the unit is entered (lines 9000-9050), then the numerical value (line 9100). Based on the unit selection, the input value (VP) is converted to a mm Hg basis (lines 9150-9175). Line 9200 computes ANSWER.

A.8.14 The Da Estimation Subroutine

The code for this routine is shown in Figure A-18. DAINFO.CMP contains the information screen and the two selection options. SLN is entered at line 9300; the temperature (TEMP) is entered at line 9375. If a rough approximation is desired (SLN = 1), the calculation occurs at line 9450.

If the FSG method (SLN = 2) is chosen, its instructions are displayed at lines 9475-9700, and the contents of LEBASA.CMP are down-loaded (lines 9725-9750). They include the 22-element string LBA\$, which contains the identification of atoms or structural constituents, the 22-element array LBAS, which contains the LeBas Volume contributions for each element in LBA\$, and the 22-element array MDW, which contains the atomic weights for atomic constituents (none of the structural constituents involve additional atoms). The tableau (see Figure 18, main text) is displayed by lines 9775-9800.

```

9275 PNTR=117:BLURB$(21)="-dainfo.cmp":SK=1:GOSUB 15400
9300 INPUT "Enter your selection: ",SLN
9325 IF SLN<>0 AND SLN<>1 AND SLN<>2 THEN PRINT PMT$(2):GOSUB 15850:GOTO 9275
9350 IF SLN=0 THEN 10425
9375 INPUT "Enter temperature of computation in Deg C: ",TEMP:TEMP=273.2+TEMP
9400 IF SLN=2 THEN GOTO 9475 ELSE GOSUB 15775
9450 ANSWER=((TEMP+1.75)/(298.2+1.75))*8/SQR(MWT):GOTO 10390
9475 PRINT "*** INSTRUCTIONS FOR LE BAS VOLUME EVALUATION (FSG METHOD) *****"
9500 PRINT "The CRT will display the FSG method structure units."
9525 PRINT "You will be prompted to enter the structural constituent"
9535 PRINT "identification number for a constituent in the pollutant."
9575 PRINT "The cursor will move to that item. There, you enter the number"
9580 PRINT "of units in the pollutant structure. For example,"
9600 PRINT "if your structure was CH2Cl-CHBr-COOH, you would enter:"
9625 PRINT "ID#1 [C] 3; ID#2 [H] 4; ID#4 [Br] 1; ID#6 [Cl],1 ; and ID #9"
9650 PRINT "[Carboxylic O] 2. At the end of each entry, you are queried"
9675 PRINT "to continue with entries, and the sequence above is repeated"
9700 PRINT "until you respond 'no' to this query.":SK=0:GOSUB 15675:CLS
9725 OPEN "LEBASA.CMP" FOR INPUT AS #1
9750 FOR J%=1 TO 23:INPUT #1,LBAS$(J%),LBAS(J%),MOW(J%):NOLB(J%)=0:NEXT J%:
CLOSE #1
9775 LOCATE 1,20:PRINT "LEBAS VOLUME CONSTITUENT UNITS"
9800 FOR J%=1 TO 11:PRINT LBAS$(2*J%-1) TAB(35) NOLB(2*J%-1)
TAB(40) LBAS$(2*J%) TAB(65) NOLB(2*J%):NEXT J%
9805 PRINT LBAS$(23) TAB(35) NOLB(23)
9850 PRINT "Enter ID# when prompted. Then cursor will move to ID# location."
9875 PRINT "At that location, enter the number of units."
10000 LOCATE 16,1:FOR J%=1 TO 4:PRINT PMT$(6):NEXT J%
10025 LOCATE 16,5:INPUT "Enter ID# of constituent here: ",NID
10050 IF NID<1 OR NID>23 THEN LOCATE 17,5:PRINT "Input is out of range."
TRY AGAIN":SK=0:GOSUB 15675:GOTO 10000
10075 IF NID>INT(NID) THEN LOCATE 17,5:PRINT "Integer input needed."
TRY AGAIN":SK=0:GOSUB 15675:GOTO 10000
10100 JLINE=1+INT((NID-1)/2)
10125 KLINE=NID MOD 2:IF KLINE=0 THEN PXOS=65 ELSE PXOS=35
10150 LOCATE JLINE+1,PXOS:INPUT;" ",NOLB(NID)
10175 IF NOLB(NID)=INT(NOLB(NID)) THEN GOSUB 10380:GOTO 10225
10180 LOCATE 16,5:PRINT "Integer input needed. Try again. ":
LOCATE JLINE+1,PXOS:NOLB(NID)=0:PRINT "0 ";GOTO 10150
10225 GOSUB 10380:LOCATE 18,1:INPUT "Do you want to do more (yes or no)? ",ANY$
10250 IF ANY$<>"yes" AND ANY$<>"no" THEN PRINT PMT$(2):SK=0:
GOSUB 15675:GOTO 10225
10275 IF ANY$="yes" THEN 9775
10300 LASUM=0:MWT=0
10305 FOR J%=1 TO 23:LASUM=LASUM+NOLB(J%)*LBAS(J%):MWT=MWT+MOW(J%)*NOLB(J%):
NEXT J%
10307 GOSUB 10380:LOCATE 18,1:PRINT "Lebas Volume = " LASUM
10310 IF LASUM <1 THEN PRINT "You probably made a mistake in LeBas Inputs."
TRY AGAIN":GOSUB 15850:GOTO 9475
10315 LOCATE 19,1:PRINT "Molecular weight computed from LeBas Volume
Inputs is "MWT
10317 IF LIMIT(5)=0 THEN 10320 ELSE LOCATE 20,1:PRINT "Mol Wt in file "
PMT$(14) " = "PANV(91)
10318 LOCATE 21,1:PRINT "If different, error either in Mol Wt in .DAT
file or LeBas inputs."
10320 LOCATE 22,1:PRINT "Temperature of computation is " TEMP-273.2 " Celcius"
10325 VOLB=.875*LASUM:VTERM=(20.1^(1/3)+VOLB(1/3))^2
10350 MRED=(28.97*MWT)/(28.97*MWT)
10375 ANSWER=8.639999E-03*TEMP^(7/4)*SQR(MRED)/VTERM:GOTO 10390
10380 LOCATE 17,1:FOR J%=1 TO 4:PRINT PMT$(6):NEXT J%:RETURN
10390 GOSUB 15800
10425 RETURN

```

Figure A-18. Da Estimation Subroutine

The data entry sequence algorithm starts with line 10025. The input prompt "Enter ID# of constituent here:" is displayed. You input the index NID, and lines 10100-10150 cause the monitor cursor to move to the right of the LBAS\$(NID) string, where you enter the number of constituents NOLB(NID). Line 10225 displays the prompt "Do you want to do more (yes or no)? to which your response

is ANY\$. If ANY\$ = yes , execution is transferred back to line 9775 to redisplay the tableau with updated information. If ANY\$ = no , the LeBas Volume (LASUM) and molecular weight (MWT) are computed at line 10300. The LeBas Volume is displayed by line 10307. If LASUM < 0 , which indicates an input error, the statement of line 10310 is displayed, and execution transfers to line 9475, to repeat the volume input process.

At line 10315, MWT is displayed. If you entered CHMPRP11 from CHMFIL11, the next display is the on-line molecular weight, PANV(91). MWT is used to compute Da. Lines 10317-10320 are the advisory message to check both entries in case there is a discrepancy greater than round-off error (atomic weights used are to the nearest 0.1 atomic unit.) ANSWER is computed at line 10375.

A.8.15 The Kd Subroutine

The code for this subroutine is in Figure A-19. The selection menu is at lines 10500-10650. Line 10710 prevents use of option 1 or 2 if LIMIT(5) = 0 ; the user is sent back to line 10500. Koc is picked up at line 10725. If SLN = 1 , the branch at line 10750 does not apply, and line 10800 causes the subroutine at line 15000 to be entered (see Figure A-16) to download the specified .LDS file. The subroutine return is to line 10825, which is also the entry point for processing for the second option. Line 10825 checks if all of the foc variables PANV(56), PANV(61), or PANV(65) are zero; if so, a message is displayed, and the user is sent back to line 10500. Lines 10875-10885 determine which foc to use of the three on-line values, and that foc is displayed at line 10890.* ANSWER is computed at line 10925, and the result printed out at line 10950.

For the last option (line 10600), execution starts at line 10900, where foc is entered. ANSWER is computed at line 10925 and the result displayed on line 10930.

A.8 16 The Cattle Toxicity Limit Subroutine

The code for this subroutine is also in Figure A-19. The informational screen and choice of options is in CATTOX.CMP. The subroutine for SLN = 1 starts at line 11350, where NOEL is input (either manually or from PANV(101)). ANSWER is computed at line 11360 and displayed at the GOSUB return line 11343. The other options are straightforward.

* See Table 1 for the foc - Kd correspondence.

```

.....Subroutine to Estimate Kd.....
10450 CLS:PRINT "***** INFORMATION ON *****"
10475 BLURBS(21)="kdinfo.cmp":SK=0:GOSUB 15550
10500 PRINT "***** SELECTION MENU TO ESTIMATE KD *****"
10525 PRINT "Select '0' to exit without any estimate performed"
10550 PRINT "Select '1' for KD from foc in .LDS file (CHMFIL11 users only!!)"
10575 PRINT "Select '2' for KD from on-line foc data (CHMFIL11 users only!!)"
10600 PRINT "Select '3' for KD based on manual input of foc value"
10625 PRINT "NOTE: If you are here from CHMFIL11, program keeps track of"
10650 INPUT "which KD you are evaluating. Enter your selection: ",SLN
10675 IF SLN<>0 AND SLN<>1 AND SLN<>2 AND SLN<>3 THEN PRINT PMT$(2):GOTO 10500
10700 IF SLN=0 THEN 10425
10710 IF LIMIT(5)=0 AND SLN<>3 THEN PRINT "Sorry, can't use this method.
      Use only '3' ":GOTO 10500
10725 IF LIMIT(5)=0 THEN INPUT "Enter Koc (SOC-water partition coeff.): ",
      KOC ELSE KOC=PANV(101):PRINT PANM$(101) " = "PANV(101)
10750 ON SLN-1 GOTO 10825, 10900
10800 GOSUB 15000
10825 IF PANV(56)<>0 AND PANV(61)<>0 AND PANV(65)<>0 THEN GOTO 10875
      ELSE PRINT "Invalid data set may exist on-line. Last down-loaded
      file is "PMT$(12)
10850 PRINT "If no file shown, no on-line data exist. If file shown,
      at least ":PRINT "one foc = 0. Either try another file or method.":
      GOTO 10500
10875 IF LIMIT(6)=28 THEN FOC=PANV(56)
10880 IF LIMIT(6)=29 THEN FOC=PANV(61)
10885 IF LIMIT(6)=30 THEN FOC=PANV(65)
10890 PRINT "The fraction organic carbon (foc) used is "FOC:GOTO 10925
10900 INPUT "Input the foc value for the soil situation in question: ",FOC
10925 ANSWER=FOC*KOC:IF LIMIT(5)=1 THEN 10950
10930 PRINT "KD = " ANSWER:RETURN
10950 PRINT PANM$(90+LIMIT(6)) " = " ANSWER:RETURN
.....Subroutine to estimate the Cattle Toxicity Constraint Limit.....
11300 PNTR=133:BLURBS(21)="catttox.cmp":SK=1:GOSUB 15400
11330 INPUT "Enter your selection (from 0 to 3): ",SLN
11335 IF SLN<>0 AND SLN<>1 AND SLN<>2 AND SLN<>3 THEN
      PRINT PMT$(2):GOSUB 15850:GOTO 11300
11340 IF SLN=0 THEN 11348 ELSE ON SLN GOSUB 11350,11400,11450
11343 GOSUB 15800
11348 RETURN
11350 IF LIMIT(5)=0 THEN INPUT "Enter Human NOEL in mg/kg-day: ",NOEL
      ELSE NOEL=PANV(101):PRINT PANM$(101) " = "PANV(101)
11360 ANSWER=NOEL*100:RETURN
11400 INPUT "Enter Mammalian Lifetime NOEL in mg/kg-day: ",NOEL
11410 ANSWER=NOEL/10:RETURN
11450 INPUT "Enter mammalian 90-day NOEL in mg/kg-day: ",NOEL
11460 ANSWER=NOEL/100:RETURN

```

Figure A-19. Estimation Subroutines for Kd and the Cattle Toxicity Constraint Limit

APPENDIX B. EQUATIONS USED TO COMPUTE UNIT CONCENTRATION INTAKES AND GLOSSARY.

The equations in Table B-1 are used in COMPUT11 to evaluate the elements of the INTAKE array. The symbols used in Table 1 correspond to of Table 1 of the main text. The in-program identification of these symbols, with units, is provided in Table B-2. Other frequently-used terms and acronyms appear in Table B-3. Certain recurring combinations of variables are defined below:

$$\begin{aligned} KD1 &= Kd1 + th1/rh1 \\ KD2 &= Kd2 + th2/rh2 \\ KD3 &= Kd3 + th3/rh3 \end{aligned}$$

TABLE B-1. INTAKE EQUATIONS

Index*	Pathway Description	Evaluation Term
<u>WATER PATHWAYS</u>		
1	Drink water	$Ww \times SWw$
2	Eat fish	$Wf \times SWf \times BCF$
3	Eat vegetables	$Wv \times SWv \times Kwv$
4	Eat beef (cows drink water)	$Wm \times SWm \times Kpm \times Uwm / Upm$
5	Eat beef (cows drink water, eat pasture)	$Wm \times SWm \times Kpm \times (Kwp + Uwm / Upm)$
6	Drink milk (cows drink water)	$Wd \times SWd \times Kpd \times Uwd / Upd$
7	Drink milk (cows drink water, eat pasture)	$Wd \times SWd \times Kpd \times (Kwp + Uwd / Upd)$
8	Skin absorption	$10 \times AV \times Teff \times PC \times S(PC) **$
<u>SOIL PATHWAYS</u>		
11	Drink water	$Ww \times SWw \times f(S1) / KD2$
12	Eat fish	$Wf \times SWf \times BCF \times f(S2) / KD2$
13	Eat vegetables	$Wv \times SWv \times Kwv / KD1$
14	Eat beef (cows eat pasture)	$Wm \times SWm \times Kwp \times Kpm / KD1$
15	Eat beef (cows eat pasture, ingest soil)	$INTAKE(31) + INTAKE(32)$
31		$Wm \times SWm \times Kpm \times Kwp / KD1$
32		$Wm \times SWm \times Kpm \times Usm / Upm$
16	Eat beef (cows eat pasture, ingest soil, drink water)	$INTAKE(31) + INTAKE(32) + INTAKE(33)$
33		$Wm \times SWm \times Kpm \times Uwm / (Upm \times KD2)$
17	Drink milk (cows eat pasture)	$Wd \times SWd \times Kwp \times Kpd / KD1$

* Index identifies elements in the INPUTS array; see Section A.7 and Figure A-6 in Appendix A.

** Constant required for unit conversions.

TABLE B-1. INTAKE EQUATIONS (concluded)

Index	Pathway Description	Evaluation Term
18	Drink milk (cows eat pasture, ingest soil)	INTAKE(34) + INTAKE(35)
34		$Wd \times SWd \times Kpd \times Kwp / KD1$
35		$Wd \times SWd \times Kpd \times Usd / Upd$
19	Drink milk (cows eat pasture, ingest soil, drink water)	INTAKE(34) + INTAKE(35) + INTAKE(36)
36		$Wd \times SWd \times Kpd \times Uwd / (Upd \times KD2)$
20	Normal soil	$Wsn \times SWSn$
21	Dusty work	$Wscw \times SWscw$
22	Diffusion from basement or enclosure	$Rb \times SRb \times TAC \times FAVN / VAR$ where: $DAS = Da \times ep3^{10/3} / (ep3 + th3)^2$ $COF1 = 1000 \times Kh / KD3 *$ $COF2 = (DAS \times [ep3 + th3/Kh + rh3 \times KD3/Kh])^{0.5}$ $FN(TOb) = TOb \times COF1 \times COF2 / (3.1416 \times TOb)^{0.5}$ $FN(TLb) = TLb \times COF1 \times COF2 / (3.1416 \times TLb)^{0.5}$ $FAVN = 2 \times FN(TOb) \times FN(TLb) / (TLb - TOb)$
23	Diffusion from open area (person on site)	$Rw \times SRw \times LS \times FAVN / (86400 \times VW \times MH) *$ where: $DAS = Da \times ep1^{10/3} / (ep1 + th1)^2$ $COF1 = 1000 \times Kh / KD1 *$ $COF2 = (DAS \times [ep1 + th1/Kh + rh1 \times KD1/Kh])^{0.5}$ See Pathway 22 for FN(TO), FN(TL), and FAVN**
24	Skin absorption from water	$10 \times AV \times Teff \times PC \times S(PC) \times f(S1) / KD2 *$

* Constant required for units conversions.

** T0o and TLo respectively replace TOb and TLb.

TABLE B-2. Listing of Variables Used in Table B-1 Equations and Other Variables from Table 1, Main Text.

Index*	Title, Units, and Symbol**
1	Adult body weight, kg [BW]
2	Child body weight, kg [BWc]
3	Representative water intake, L/day [Ww]
4	Representative fish intake, kg/day [Wf]
5	Representative vegetable intake, kg dwb*** /day [Wv]
6	Representative beef intake, kg/day [Wm]
7	Representative dairy intake, L/day [Wd]
8	Incidental soil ingestion rate, normal conditions, kg/day [Wsn]
9	Incidental soil ingestion rate, dusty conditions, kg/day [Wscw]
10	Inhalation rate, enclosed area vapor model, m ³ /day [Rb]
11	Inhalation rate, open area vapor model, m ³ /day [Rw]
12	Body surface area for dermal exposure, m ² [AV]
13	Effective daily exposure to dermal contaminant, hr [Teff]
14-22	Not used
23	Adjustment for less than representative water intake [SWw]
24	Adjustment for less than representative fish intake [SWf]
25	Adjustment for less than representative vegetable intake [SWv]
26	Adjustment for less than representative beef intake [SWm]
27	Adjustment for less than representative dairy intake [SWd]
28	Adjustment for non-model exposure to soil/dust [SWsn]
29	Adjustment for non-model worksite conditions [SWscw]
30	Adjustment for tenure in enclosed area vapor model [SRb]
31	Adjustment for tenure in open area vapor model [SRw]
32	Not used
33	Adjustment for tenure in exposure to bath water [S(PC)]
34-40	Not used
41	Fat content of beef, fraction [fm]
42	Fat content of milk, fraction [fd]
43	Steer uptake of water, L/day [Uwm]
44	Steer uptake of forage, kg dwb/day [Upm]
45	Steer incidental uptake of soil in forage, kg/day [Usm]
46	Dairy cow uptake of water, L/day [Uwd]
47	Dairy cow uptake of forage, kg dwb/day [Upd]
48	Dairy cow incidental uptake of soil in forage, kg/day [Usd]
49	Time average body weight of steer, kg
50	Weight of dairy cow in milk production, kg
51-55	Not used
56	Surface soil organic carbon fraction [foc1]
57	Surface soil nominal density, kg/L [rh1]
58	Surface soil moisture content, fraction [th1]
59	Soil to water dilution factor for oral/dermal water source [f(S1)]
60	Soil to surface water dilution factor for fish pathways [f(S2)]

* Index identifies elements in the PANM\$ array; see Table A-1 in Appendix A.

** These descriptions can also be found in the file PARAM.CMP.

*** dwb = dry weight basis.

TABLE B-2. Listing of Variables Used in Table B-1 Equations and Other Variables from Table 1, Main Text (continued).

Index	Title, Units, and Symbol
61	Drinking water body sediment organic carbon fraction [foc2]
62	Drinking water body sediment nominal density, kg/L [rh2]
63	Drinking water body sediment moisture content [th2]
64	Vapor-laden top-soil representative void fraction [ep1]
65	Vapor-laden soil representative org. carbon fraction [foc3]
66	Vapor-laden soil representative bulk density, kg/L [rh3]
67	Vapor-laden soil representative moisture content [th3]
68	Vapor-laden soil representative void fraction [ep3]
69-75	Not used
76	Volume-area ratio of basement(or other enclosure), m [VAR]
77	Time per air change factor for enclosure vapor path, days [TAC]
78	Windspeed at open-air site, m/sec [VW] (1m/sec = 2.24mph)
79	Height in which mixing occurs at open-air site, m [MH]
80	Initial time of analysis(entry), basement diffusion case, day [TOb]
81	End time of analysis, basement diffusion case, day [TLb]
82	Representative area length, m [LS]
83	Initial time of outside soil diffusion case, day [T0o]
84	End time of outside soil diffusion case, day [TLo]
85-90	Not used
91	Molecular weight, g/gmol [MW]
92	Normal or extrapolated melting point, deg C [Tmelt]
93	Normal or extrapolated boiling point, deg C [Tboil]
94	Log octanol-water partition coefficient [LogKow]
95	Water solubility, mg/L [SW]
96	Saturated vapor pressure, mm Hg [VP]
97-100	Not used
101	Soil organic carbon (OC) to water p.c.*, L water/kg OC [Koc]
102	Soil to forage partition coefficient, kg soil/kg dwb forage Ksp
103	Soil to vegetable partition coefficient, kg soil/kg dwb [Ksv]
104	Reference soil foc for Ksp measurement.
105	Reference soil foc for Ksv measurement.
106	Forage to meat fat p.c., kg dwb forage/kg adipose tissue [Kpat]
107-110	Not used
111	Fish bioconcentration factor, L/kg fish [BCF]
112	Water to vegetable partition coefficient, L/kg dwb [Kwv]
113	Water to forage partition coefficient, L/kg dwb forage [Kwp]
114	Plant to beef partition coefficient, kg dw forage/kg meat [Kpm]
115	Plant to dairy partition coefficient, kg dwb forage/L milk [Kpd]
116	Henry Law constant, dimensionless [Kh]
117	Molecular diffusivity in air, m ² /day [Da]
118	Soil to water partition coefficient, surface soil, L/kg [Kd1]
119	Soil to water partition coefficient, sediment, L/kg [Kd2]
120	Soil to water p.c., mixed surface/subsurface soil, L/kg [Kd3]
121	Dermal permeability constant, cm/hr [PC]
122-125	Not used

* p.c. = partition coefficient

TABLE B-2. Listing of Variables Used in Table B-1 Equations and Other Variables from Table 1, Main Text (concluded).

Index	Title, Units, and Symbol
126	Long term no-effect human dose, mg/kg-day [DT]
127	Shorter term no-effect human dose, mg/kg-day [DTc]
128-130	Not used
131	Organoleptic taste limit in water, mg/L
132	Constraint to avoid damage to aquatic biota systems, mg/L
133	Acceptable limit dose to cattle, mg/kg-day
134	Phytotoxic limit in hydroponic solution, mg/L
135	Phytotoxic limit in soil, mg/kg
136	Fraction organic carbon of soil used in phytotoxicity study
137-140	Not used

Table B-3. Frequently-Used Terms and Acronyms.

array - A name associated with several variables (elements), each distinguished by a numerical identification (index)

BASIC - Programming language used in PHAS (Microsoft GW-BASIC)

CHMFIL11 - Program used to prepare chemical-specific data, and handle .DAT files for use, storage, or modification

CHMPRP11 - Program used to provide information about chemical properties and selected estimation methods

COMMON - Command used to designate variables for use in two or more programs by the same name

.CMP - Extension for file used to store down-loaded data or verbal descriptions to programs within PHAS

COMPUT11 - Program used to perform PPLV and constraint analyses

current session - All transactions in PHAS since the command to start execution to the current time

.DAT - Extension for file used to store chemical-specific data

DIM - A BASIC command to designate the number of elements in an array

DOS - Disk Operating System (Microsoft MS-DOS, Version 3.3) for IBM personal computers and compatible hardware systems

down-load - Transfer of information from a file in storage to program memory

DUST - Data Use Status Table

dwb - Dry weight basis

element - A specific member of an array

FIN - Fragment identifier number

GOSUB - A command to transfer execution to a specific line of a program. The process ends with a RETURN, which transfers control to the line following the GOSUB command.

GOTO - A command to transfer execution to a specific line of a program

Table B-3. Frequently-Used Terms and Acronyms.

index - A number which identifies a particular element of an array
INPUTS11 - Program used to prepare non-chemical specific data, and handle .LDS files for use, storage or modification
INSTALL - Program used to identify the device where .DAT, .LDS , and .PTH file will be located when PHAS is executed.

.LDS - Extension for file used to store non-chemical specific data

on-line storage - Information in program memory identified by common variables and accessible by any PHAS module

OPEN11 - Program used to enter and exit PHAS, switch between other programs, review on-line data, and read advisory messages about the system

PATWAY11 - Program used to prepare scenario information, and prepare .PTH files for use or storage

p.c. - Partition coefficient

PHAS - Pollutant Hazard Assessment System

.PTH - Extension for file used to store scenario information

PPLV - Preliminary Pollutant Limit Value

RETURN - The BASIC command to transfer to the line after a GOSUB call

SPLV - Single Pathway Limit Value

string - A variable whose contents are taken to be alphanumeric (usually words)

subroutine - A series of commands which are directed by a GOSUB and is ended by a RETURN

variable - A name assigned to a datum for processing in a program

APPENDIX C. VALUES OF VARIABLES IN THE FILES DEFALVA.LDS AND DEFALVC.LDS

Variable and Index	Value*	Comment
BW (1)	70 kg	See Small ¹² , section 5.1.1.1.
BWc (2)	12 kg	Based on rounded-off mean weights of 2-year old male and female children, see Table 8, Small ¹² .
Ww (3)	1.6 L/day (DEFALVA)** 1 L/day (DEFALVC)**	See Small ¹² , section 5.1.2. As noted, 1.0 L/day for children tends to be on the "high" side, representative of summer intake.
Wf (4)	0.0065 kg/day (DEFALVA) 0.0022 kg/day (DEFALVC)	See Small ¹² , section 5.1.3. EPA uses 6.5 g/day for Water Quality Criteria, which is a per-capita intake of fresh and estuarine fish. However, value probably also approximates freshwater intake of per-capita individuals. Intake in DEFALVC is one-third of adult value; approximate ratio of average fish intake by 0-9 year-olds to adults.
Wv (5)	0.017 kg/day (DEFALVA) 0.008 kg/day (DEFALVC)	See Small ¹² , section 5.1.4 and Table 13. Adult value (0.017 kg/day) is estimated per-capita intake for "rural non-farm" locales. Child intake pro-rated based on potato, other vegetable and fruit intakes in Table 9 of Small ¹² (about 45 percent). These weights are on a dry-weight basis.
Wm (6)	0.1 kg/day (DEFALVA) 0.04 kg/day (DEFALVC)	Adult intake, see Small ¹² , section 5.1.5. Child intake pro-rated based on data in Table 9 of Small ¹² (about 42 percent).
Wd (7)	0.3 L/day (DEFALVA) 0.56 L/day (DEFALVC)	Adult intake, see Small ¹² , section 5.1.6. For child intake, see Table 9.

* See Appendix B, Table B-2 for units.

** For brevity, the .LDS extension has been omitted.

APPENDIX C. VALUES OF VARIABLES IN THE FILES DEFALVA.LDS AND DEFALVC.LDS

Variable and Index	Value	Comment
Wsn (8)	7.4e-5 kg/day (DEFALVA) 8.2e-4 kg/day (DEFALVC)	See Small ¹² , section 5.1.8 for development of adult value. Note that this is a time-averaged value over a lifetime. In DEFALVC, the value is from Table 15 for the 2-3 year old interval.
Wscw (9)	1.8e-4 kg/day (DEFALVA) 0 (DEFALVC)	See Small ¹² , section 5.1.9 for development of adult value. Note that specific oral and inhalation intakes are involved (a total of 400 mg/day), as well as an assumed 44 percent occurrence of "dusty" conditions per year. Since children are not expected at work sites, zero is in the DEFALVC file.
Rb (10)	1.5 m ³ /day (DEFALVA) 0.75 m ³ /day (DEFALVC)	Adult value based on 1.2 hours/day exposure to vapors in basement and inhalation rate of 1.2 m ³ /hour. Child value assumed to be one-half that of an adult.
Rw (11)	17 m ³ /day (DEFALVA) 0 (DEFALVC)	Value is for adult male inhalation for 8 hours under "moderate" exertion conditions; see Small ¹² , section 5.1.7. Child rate is not applicable to work sites.
AV (12)	1.8 m ² (DEFALVA) 0.72 m ² (DEFALVC)	Adult value is average of full male and female body ¹¹ . Child value is based on cite for average 3- to 6-year old child ¹¹ .
Teff (13)	1 hr/day	Default value. Valuation will depend upon specific exposure activity. For example, outdoor swimming or bathing time has been estimated at 2.6 hr per event day; baths or showers at about 15 minutes ⁵ .
"S- (23-33) adjustment factors"		These factors are set to unity. User's judgement is required for based on problem-specific factors.
fm (41)	0.25	See Small ¹² , section 5.2.6; choice meat basis.

APPENDIX C. VALUES OF VARIABLES IN THE FILES DEFALVA.LDS AND DEFALVC.LDS

Variable and Index	Value	Comment
fd (42)	0.04	See Small ¹² , section 5.2.6.
Uwm (43)	15.3 L/day	See Small ¹² , section 5.2.2. Based on 0.055 L/kg-day intake time averaged over a modelled steer's lifetime. For rapidly-metabolized substances, a 400 kg weight basis (22 L/day) should be more appropriate.
Upm (44)	6.6 kg/day (dry weight basis)	See Small ¹² , section 5.2.1. Based on modelled feeding schedule. For rapidly-metabolized substances, a 25 g/kg-day intake for a 400 kg steer or 10 kg/day should be more appropriate.
Usm (45)	0.35 kg/day	See Small ¹² , section 5.2.5. Based on soil comprising 5% of total diet (Upm comprises the other 95%). For rapidly-metabolized substances, an intake of 0.53 kg/day should be more appropriate.
Uwd (46)	78 L/day	See Small ¹² , section 5.2.4.
Upd (47)	16.6 kg/day (dry weight basis)	See Small ¹² , section 5.2.3.
Usd (48)	0.87 kg/day	See Small ¹² , section 5.2.5.
Steer (49)	250 kg	See Small ¹² , section 5.2.1. Time-weighted averaged weight. For rapidly-metabolized substances, a 400 kg weight should be more appropriate.
Dairy cow weight(50)	520 kg	See Small ¹² , section 5.2.3.
foc1 (56)	0.02	Default value; see Small ¹² , section 5.3.2.

APPENDIX C. VALUES OF VARIABLES IN THE FILES DEFALVA.LDS AND DEFALVC.LDS

Variable and Index	Value	Comment
rh1 (57)	1.4 kg/L	Default value, based on 55% of topsoil volume as solids (water and air occupy voids) and 2.6 g/cc density of voidless solids.
th1 (58)	0.1	Default value; see Sma11 ² , section 5.3.1.
f(S1) (59)	1	These factors are set to unity. User's judgement is required for adjustment based on problem-specific factors.
f(S2) (60)		
foc2 (61)	0.1	Default value.
rh2 (62)	1.4 kg/L	Default value; see rh1.
th2 (63)	0.4	Default value; see Sma11 ² , section 5.3.1.
ep1 (64)	0.25	Default value; see Sma11 ² , section 5.3.1.
foc3 (65)	0.001	Default value; see Sma11 ² , section 5.3.2.
rh3 (66)	1.6 kg/L	Default value; see Sma11 ² , section 5.3.1.
th3 (67)	0.2	Default value; see Sma11 ² , section 5.3.1.
ep3 (68)	0.2	Default value; see Sma11 ² , section 5.3.1.
VAR (76)	1.34 m	Default value; see Sma11 ² , section 5.3.3.
TAC (77)	0.083 days	Default value; see Sma11 ² , section 5.3.3.
VW (78)	2 m/sec	Default value; see Sma11 ² , section 5.3.4.
MH (79)	20 m	Default value; see Sma11 ² , section 5.3.4.

APPENDIX C. VALUES OF VARIABLES IN THE FILES DEFALVA.LDS AND DEFALVC.LDS

Variable and Index	Value	Comment
TOb (80)	60 days	Default value; see Small ² , section 5.3.5.
TLb (81)	25600 days	Default value; see Small ² , section 5.3.5.
LS (82)	100 m	Default value; see Small ² , section 5.3.4.
T0o (83)	0.01 day	Default value; see Small ² , section 5.3.5.
TLo (84)	1 day	Default value; see Small ² , section 5.3.5.

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